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Redstone Arsenal, Alabama 35809



TECHNICAL REPORT H-78-1

COMPILATION OF DATA RELEVANT TO NUCLEAR PUMPED LASERS

VOLUME III

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December 1978

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ABSTRACT (CONCLUDED)

Volumes III, IV, and V contain data on many different species of atoms, molecules, and ions: a large fraction of them are already of direct interest in laser media; many more may become important in the future. These volumes cover all of the subjects treated in Vols. I and II; one difference is that now secondary electron energy spectra are discussed in a separate chapter. A chapter on nuclear data has also been added.

A species index for all five volumes will be published separately.



PREFACE

This volume, and the succeeding Volumes No. IV and V, contain a compilation of data relevant to nuclear pumped lasers and are part of a series on atomic and molecular data for gas laser research and development. The first two volumes, published as MIRADCOM Technical Report H-78-1 in December 1977, contained "Compilation of Data Relevant to Rare Gas-Rare Gas and Rare Gas-Monohalide Excimer Laser" by E. W. McDaniel, M. R. Flannery, H. W. Ellis, F. L. Eisele, W. Pope, and T. G. Roberts. These first two volumes are referred to herein as "Vol. I" and "Vol. II," usually without further designation.

In Vols. I and II, heavy emphasis was placed on the rare gases and halogens (atoms, molecules, and ions), and on the rare gas-halides, although a significant amount of material on other species was included. Vol. I deals with structural properties and with heavy particle-heavy particle collisions. Vol. II treats the collisions of electrons and photons with heavy particles; transport properties of electrons, ions, and neutrals; interactions of heavy particles with electric and magnetic fields; particle penetration in gases; and particle and photon interactions with solids.

Vols. I and II were prepared in the context of the two most-used techniques for gas laser pumping: electrical discharges and high intensity, high energy electron and ion beams. Vols. III, IV, and V contain much information relevant to electrical discharges and high intensity, high energy electron and ion beams, but are oriented toward a third pumping technique: nuclear pumping. This mechanism involves direct nuclear excitation of the laser gas in which, for example, a pulsed nuclear reactor generates a high intensity pulse of neutrons of duration between 0.1 and 10 msec. These neutrons produce fission in reactions with heavy nuclides within the laser or interact with light nuclides in (n,p) or (n,α) reactions. The high energy charged particles thus produced then deposit their energy in excitation and ionization of the laser gas in reactions similar to those taking place when a high energy electron beam traverses the laser. Nuclear pumping has been achieved with He, Ne, Ar, Kr, Xe, C, N, O, Hg, CO, mixtures of the rare gases, and possibly with CO2, KrF, and XeF. These nuclear reactions may also become interesting in some form of a hybrid laser where the excitation and ionization produced might be used to supply electrons for an electrical discharge laser or an initiator for a pulsed chemical laser, or as an initiator and sustainer for a continuous wave (CW) chemical laser. Therefore, some data relevant to those systems have also been included.

The laser pumping mechanisms, when viewed on the molecular level, are frequently extremely complex. Some inkling of this situation is provided by consideration of the bizarre combinations of gases often

used in lasers to produce and/or pump the atomic or molecular species of interest. Some of these combinations are as unexpected, felicitous, and efficacious as that of lox, bagels, and cream cheese. In these volumes, data on many different species of atoms, molecules, and ions are provided: a large fraction of them are already of direct interest in laser media; many more may become important in the future. This volume and the succeeding volumes cover all of the subjects treated in Vols. I and II; one difference is that now secondary electron energy spectra are discussed in a separate chapter. A chapter on nuclear data has also been added.

A species index for all five volumes will be published separately.

ACKNOWLEDGMENTS FOR VOLUME III (CHAPTER A)

The generous contribution made to this volume by Professors Stanley Bashkin and John O. Stoner of the University of Arizona who supplied the 228 atomic energy level and Grotrian diagrams used in Section A-1 is acknowledged. They also supplied most of the references that appear in Section A-2.

Special thanks are due to Dr. Nick Winter of the Lawrence Livermore Laboratories and to Dr. W. R. Wadt and Dr. P. Jeffrey Hay of the Los Alamos Scientific Laboratory for providing material for Chapter A in advance of its publication.

Drs. J. T. Moseley, D. Heustis, R. E. Olson, R. Saxon, and P. Jullienne provided much useful information on the subject of interaction potentials.

Professor W. Carl Lineberger gave expert advice on electron affinities that was much appreciated. Dr. R. D. Cowan kindly supplied information on the spectrum of the uranium atom.

Finally, we wish to thank Dr. Edward L. Wilkinson, Mr. John E. Hagefstration, and Dr. J. R. Fisher of the Ballistic Missile Advanced Technology Center for their support and encouragement during the preparation of this report.

A. STRUCTURAL PROPERTIES OF ATOMS, MOLECULES, AND IONS

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Element	Symbol	Atomic number	Atomic weight†	Element	Symbol	Atomic number	Atomic weight
Actinium	Ac	89	227	Mendelevium	Md	101	[256]
Aluminum	Al	13	26.98	Mercury	Hg	80	200.61
Americium	Am	95	[243]:	Molybdenum	Mo	42	95.95
Antimony	Sb	51	121 76	Neodymium	Nd	60	144 .27
Argon	A	18	39.944	Neptunium	Np	93	[237]
Arsenic	As	33	74.91	Neon	Ne	10	20.18
Astatine	At	85	[210]	Nickel	Ni	28	58.69
Barium	Ba	56	137.36	Niobium			
Berkelium	Bk	97	[247]	(Columbium)	Nb	41	92.91
Beryllium	Be	4	9.013	Nitrogen	N	7	14.00
Bismith	Bi	83	209.00	Nobelium	No	102	[256]
Boron	В	5	10.82	Osmium	Cis	76	190.2
Bromine	Br	35	79.916	Oxygen	0	8	16
Cadmium	Cd	48	112.41	Palladium	Pd	46	106.7
Calcium	Ca	20	40.08	Phosphorus	P	15	30.97
Californium	Cf	98	[249]	Platinum	Pt	78	195.23
Carbon	C	6	12 011	Plutonium	Pu	94	[242]
Cerium	Ce	58	140 13	Polonium	Po	84	210
Cesium	Cs	55	132 91	Potassium	K	19	39.10
Chlorine	CI	17	35.457	Praseodymium	Pr	59	140.92
Chromium	Cr	24	52.01	Promethium	Pm	61	[145]
Cobalt	Co	27	58.94	Protactinium	Pa	91	231
Columbium				Radium	Ra	88	226.05
(see Niobium) '				Radon	Rn	86	222
Copper	Cu	29	63 54	Rhenium	Re	75	186.31
Curium	Cm	96	[247]	Rhodium	Rh	45	102 91
Dysprosium	Dy	66	162 46	Rubidium	Rb	37	85.48
Einsteinium	Es	99	{254}	Ruthenium	Ru	44	101 1
Erbium	Er	68	167.2	Samarium	Sm	62	150.43
Europium	Eu	63	152.0	Scandium	Sc	21	44.96
Fermium	Fm	100	[253]	Selenium	Se	34	78.96
Fluorine	F	9	19.00	Silicon	Si	14	28.09
Francium	Fr	87	[223]	Silver	Ag	47	107 . 886
Gadolinium	Gd	64	156.9	Sodium	Na	11	22.99
Gallium	Ga	31	69.72	Strontium	Sr	38	87.63
Germanium	Ge	32	72.60	Sulfur	S	16	32.06
Gold	Au	79	197.0	Tantalum	Ta	73	180.95
Hafnium	Hf	72	178 6	Technetium	Tc	43	[99]
Helium	He	2	4.003	Tellurium	Te	52	127 61
Holmium	Ho	67	164.94	Terbium	Tb	65	158.93
Hydrogen	H	1	1.0080		Tl	81	204.39
Indium	In	49	114.76	Thorium	Th	90	232.05
Iodine	I	53	126.91	Thulium	Tm	69	168.94
Iridium. t	Ir	77	192.2	Tin	Sn	50	118.70
Iron	Fe	26	55.85	Titanium	Ti	22	47.90
Krypton	Kr	36	83 80	Tungsten	W	74	183.92
Lanthanum	La	57	138.92	Uranium	U	92	238.07
Lawrencium	Lr	103	[257]	Vanadium	v	23	50.95
Lead	Pb	82	207.21	Xenon	Xe	54	131.3
Lithium	Li	3	6.940	Ytterbium	Yb	70	173.04
Lutetium	Lu	71	174.99	Yttrium	Y	39	88.92
Magnesium	Mg	12	24.32	Zinc	Zn	30	65.38
Manganese	Mn	25	54.94	Zirconium	Zr	40	91.22

[†] Atomic weights are from the Committee on Atomic Weights of the American Chemical Society,

J. Am. Chem. Soc., 76: 2033 (1954).

‡ Atomic weights in brackets represent the isotope of longest known half-period.

Tabular Data. A-1.2. Periodic table of elements.

Orbit	M		K-L		K-L-M		Y-W-7-		131.30 -18-18-8 -M-N-O	4-0-N-	940
	He + 0028	Ne Ne	20.183	+++ 18 +5 Ar	39.948	2 X	83.80 -9-19-8	+++ Xe	131.30	86 ° Rn (22) -32-18-8	
		- E4	18.984		35.453 2-8-7	14 35 14 15 15 15 15 15 15 15 15 15 15 15 15 15	79.909		126.9044	7	
		°0		S 1211	32.064	153 Se 155	78.96	+3 52 +4 53 +5 Te +5 I	127.60	+3 84 +2 85 +5 Po +4 At 0 (210) (210) -5 (22-18-6 -32-1	
		-FFFFF	4.0067 -2	13 S 15	30.9738		74.9216		121.75	7.19 208.990 2-18-4 -32-18-5	
		777 • O	12.01115 14.0067 -2 15.9994 2-4 2-5 -3 2-6	Si ++ 15	28.086	32 +2 33 Ge +4 As	72.59 -8-18-4	Sn +2 51	18.69	1 00 DL 8 7	
		7 10 M	10.811	13 +3 14 Al Si	26.9815	+231 +332 Ga Ge	69.72	49 +3 50 In Sn	102,905 106.4 107.870 112.40 114.82 118.69 -18-16-1 -18-18-0-18-18-1 -18-18-2 -18-18-3 -18-18-4	77 77	
9				Transition	,,,,		-9-19-2	+1 48 +2 49 Cd In	112.40	Hg +1 200.50	
9				Fem		+2 29 +1 30 +3 Cu +2 Zn		47 +1 Ag +1	107.870	Au +3	
					1	28 Ni ++	38.71 63.54 -\$-16-2 -\$-18-1	45 +3 46 +747 Rh Pd +4 Ag	106.4	78 Pt ++	
	ART	← Bleetroa Coafguration			Group 8	+2 27 +2 28 +3 Co +3 Ni	58.932 -8-15-2	34 TA	102.905	17 + 14 11 11 11 11 11 11 11 11 11 11 11 11	
	← Oxidation States KEY TO CHART	Jectros Co		,	1	Fe ++	35.847 -\$-14-2	Tc + Ru	(99) -18-13-2 -18-15-1	50 S	
0,	++ x x x			Transition Elements		1 +2 24 +2 25 +2 26 + +3 Cr +3 Mn+3 Fe +	54.538 4-13-2	15 T	-1-18-13-	2 Re + + + + + + + + + + + + + + + + + +	
8	Sn ++	1911		Transit		75	51.996 2 -8-13-1	12 42 4 Mo	-1-18-13	W 183.85	
8	Atomic Number -	Avonic weignt				**** ****	47.90 50.942 -8-10-3 -8-11-2	+41 +342 +943 Nb +5 Mo Tc	91.22 -18-10-2 -18-12-1 -18-13-1	Ta Ta 188.24	
•	Atomic	486				12		+3 46	6 91.22 -2 -18-10	+3 72 Hf Hf 113.49	.77
2		7 .	9.0122	12 +1 Mg +1	24.312	Ca +221	40.08 44.966	254	87.62 88.905 -18-8-2 -18-9-2	55 +156 +257 +372 +473 +474 +475 +476 +4177 +478 +4779 +180 +1811 CS Ba La Hf Ta W Re +708 +41r +4Pt +4Au +3Hg +2TI 132.06 13734 13841 17849 180.38 180.2 180.2 180.2 180.0 180.87 20.38 204.1 189.41 189.41 180.00 180.87 20.38 204.1 189.41 189.42 10.0 180.87 20.38 204.1 189.41 189.42 10.0 180.87 20.38 204.1 189.41 189.42 10.0 180.87 20.38 204.1 189.41 189.42 10.0 180.87 20.38 204.1 189.41 189.42 10.0 180.87 20.38 204.1 189.41 1	Fr Ra Ac +3 (223) (226) (227) -18-9-1 -19-9-2
	H -1 1.00797	Li He	6.939 9.0 2-1 2-2	11 + 12 Na Mg	22.9898 24.	15 +1 28 C. C. C.	39.702 40.	37 +138 +23 Rb Sr	18-8-1	1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 +	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1

Nd H	**	PH +	Sm +3 150.35	Eu +3	Gd +3	25 25 55 55 55 55 55 55 55 55 55 55 55 5	Dy +1	58 +359 +360 +361 +362 +263 +264 +365 +366 +367 +3 Ce +49r Nd Pm Sm +3 Eu +3 Gd Tb Dy Ho 160.12 100.07 144.34 (143) 150.35 151.54 152.35 153.54 152.00 154.30 119-2.2 20-2-2 22-3-2 24-3-2 24-4-2 23-4-2 24-4-2 24-4-2 23-4-2 23-4-2	8 H 2 5 8	P P S	44 49 44 44 44 44 44 44 44 44 44 44 44 4	+271 +3 +3 Lu +3 Lu +3 -32-52
20	1777	Np+	Pr	A H	C H	90 +191 +592 +393 +394 +395 +396 +397 +398 +399 Th Pa +1 U +3 Np +3Pu +3 Am +3 Cm Bk +1 Cf Es	# %	E S	8 H	Md Md	102	103 Lw
238.00	7 7	20-02	22.038 (231) 28.03 (237) (242) (19.9-2 -20-9-2	24.92	-25-9-2	-26-9-2	(251)	254)	30-6-2	(347) (349) (351) (354) (359) (353) (359) (-31-9-3	(254)	_

(umbers in parentheses are mass numbers of most stable isotope of that element.

Notes on the Use of Energy Level and Grotrian Diagrams (Based on book by Bashkin and Stoner)

Two types of diagrams have been indispensable since their first appearance in the literature of atomic structure: energy-level diagrams and electronic transition (Grotrian) diagrams.

Energy-Level Diagrams

The general format of these diagrams is quite standard — a level is represented by a short, horizontal line which is located by two coordinates. The ordinate is the level's energy, always given in inverse centimeters [cm⁻¹], and the abscissa indicates a combination of orbital and spin angular momenta quantum numbers. The notation adhered to is primarily that of Kelly's with the adoption of the "primed" convention consistent with Moore 2.

To clarify the diagrams, each system is exhibited in a format best suited for it. For example, when energy-level densities are inconveniently high, the topmost levels are indicated together with all lower levels having a reasonable density.

The full precision of the latest experimental energy-level values has been retained and is exhibited on the diagram. In general, theoretically calculated values are shown with less precision than is given in the original sources.

The primary data on which the diagrams are based were taken primarily from Kelly's 1 exhaustive tabulations and several other references $^{2-5}$. In addition to these general references, several other references are cited for many of the systems.

Several instances occur in which ions possessing various core configurations result in many different final configurations. When this occurs, each core is given a separate diagram — specifically differentiated from the others in the title and corner labels.

Each energy-level diagram contains (1) a key which defines various symbols, (2) the ionization level (from Kelly and Palumbo 3), and (3) the ground configurations of the ion and the next higher ion. The j- ℓ and j-j intermediate coupling schemes are respectively represented by [] and $\{$ $\}$. All energy-levels and j-values are listed in order of increasing excitation. When intermediate coupling occurs, the intermediate-coupling angular momenta are shown in a vertical array in order of

increasing excitation, from bottom to top. In cases where a single energy occurs for two or more j-values, the following notation has been adopted.

For example: 797270 3d ([5/2, 3/2], 1/2),

which means that the lower level is common to the first two j-values and the upper level belongs to j = 1/2.

The ionization level is shown as a horizontal dashed line. The ionization level is simply the energy difference between the ground term and the bottom of the continuum for the terms having the ground-term core.

Grotrian Diagrams

Diagrams showing transitions from one spectroscopic term to another are called "Grotrian Diagrams." Most of the transitions have been extracted from the listing of Kelly and Palumbo³ and Striganov and Sventitskii⁴. A few others were taken from later publications. When line densities became too great for clarity, the line of shortest wavelengths together with as many of the other lines as could be conveniently drawn, were included. Lines that were omitted were selected bitrarily. In some cases, the diagram was divided into two or more diagrams. In most cases, the same energy scales were used for both the Grotrian and energy-level diagrams.

The full precision with which wavelengths have been measured has not been incorporated into the diagrams. Usually, the precisions illustrated on the diagrams is one significant figure less than that occurring in the literature. When two lines occur in a multiplet, two numbers are given, separated by a comma. When more than two lines occur, the extreme wavelengths are given, separated by a dash. Wavelengths are in vacuum for values shorter than 2000 $\overset{\text{O}}{\mathbf{A}}$ and in air for longer values.

Hyperfine effects, radio-frequency spectroscopy, and inner-shell transitions have been, for the most part, neglected.

Acknowledgments

The up-to-date enery-level and Grotrian diagrams contained herein have been provided by Stanely Bashkin⁶ and John O. Stoner, Jr., who are directing an extensive compilation project at the University of Arizona. Complete information on all neutral atoms and positive ions through Titanium XXII is presently available in three of their publications ^{7,8,9}

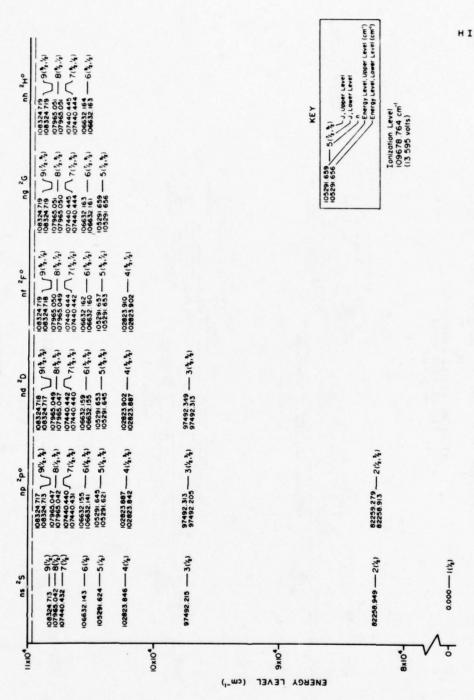
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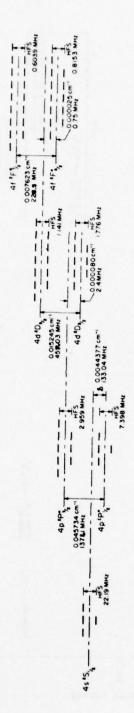
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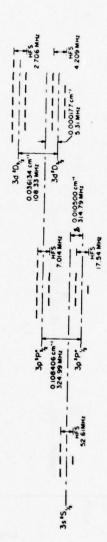
нІ			
	nh 2Ho		
	02 gn		
iron, 2=1)	nt 2F o	10936 6(%) 10936 6(%) 10936 6(%) 10936	
H I ENERGY LEVELS (1electron, 2=1) (Configuration:n1)	O ₂ Pu	1 (1) (1) (1) (1) (1) (1) (1) (1) (1) (1	
H I ENE	np ² P°	0(4, 3) 1 (4, 3	
	25		(4,1)
		ENERGY LEVEL (cm²)	-0

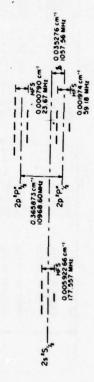
H I ENERGY LEVELS (lelectron, Z=1) (Configuration: n1)



H I ENERGY LEVELS (Lelectron, Z=1)
F.S., H.F.S., LAMB SHIFTS
(NOT TO SCALE)



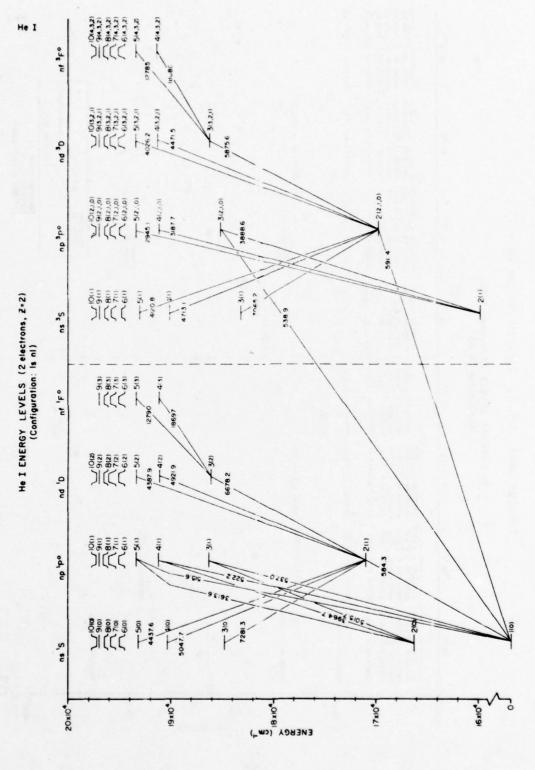






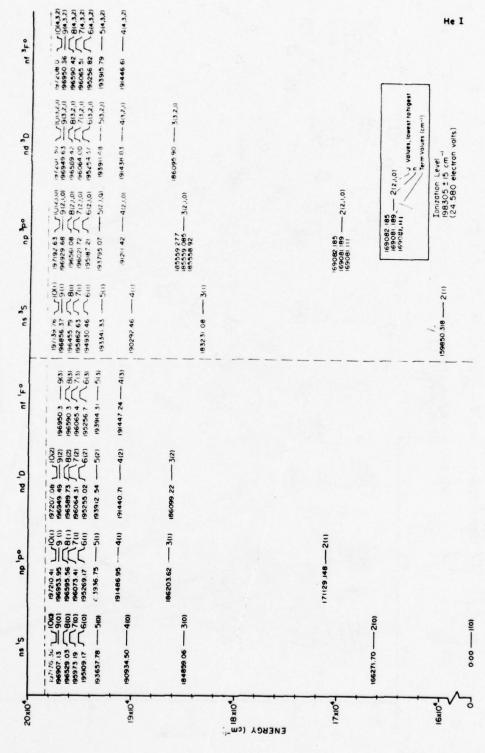
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B N Toylor, W.H. Power, D.N. Longenberg, Rev. Mad. Phys. 4, (1965)
T.

Tabular Data. A-1.6. Diagram for He (Z = 2).



Tabular Data. A-1.7. Diagram for He (Z = 2).

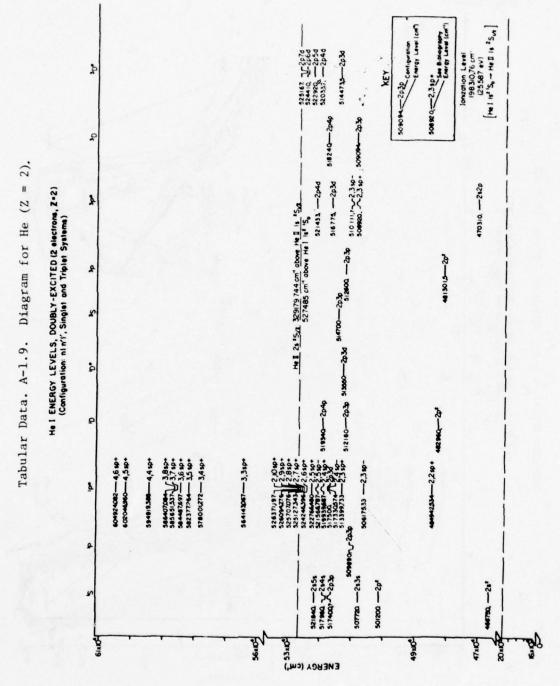
He I ENERGY LEVELS (2 electrons, Z=2) (Configuration: Is nl)



R Tabular Data. A-1.8. Diagram for He (Z = 2). He I GROTRIAN DIAGRAM, DOUBLY-EXCITED (2 electrone, Z=2) (Configuration: n1 n1', Singlet and Triplet Systems) à å 0 -2040 -2030 47x10-ENERGY (cm.1)

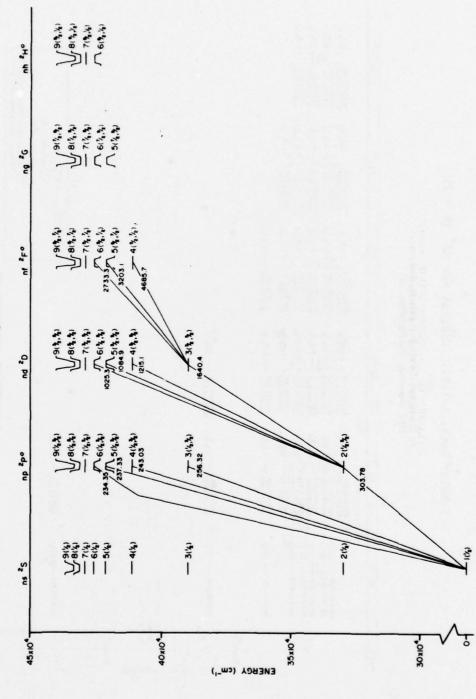
He I DOUBLY EXCITED SINGLET TRIPLET GROTRIAN DIACHAM

He I DOUBLY EXCITED SINGLET, TRIPLET



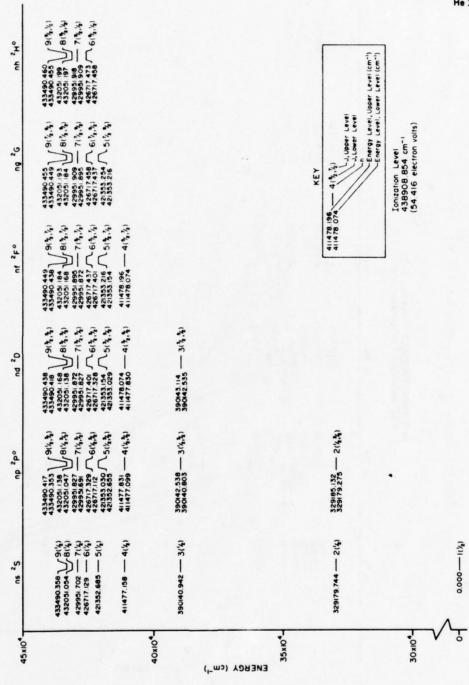
He II ENERGY LEVELS (1electron, Z=2) (HI sequence, Configuration: n1)

HeI

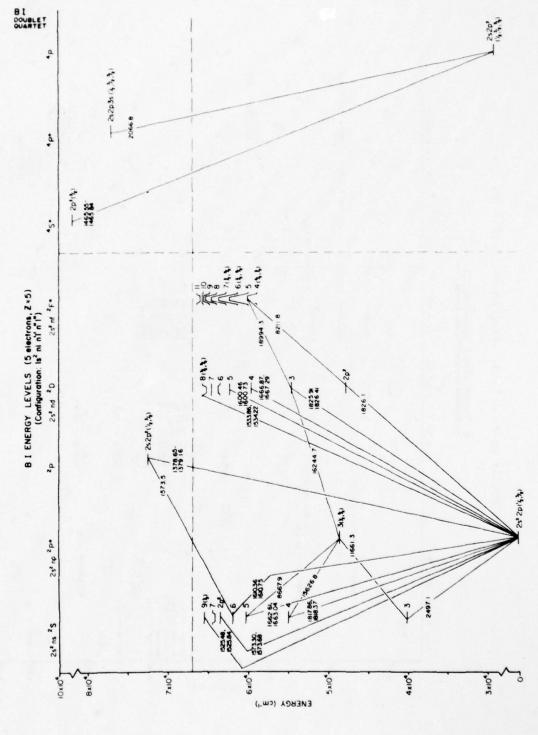


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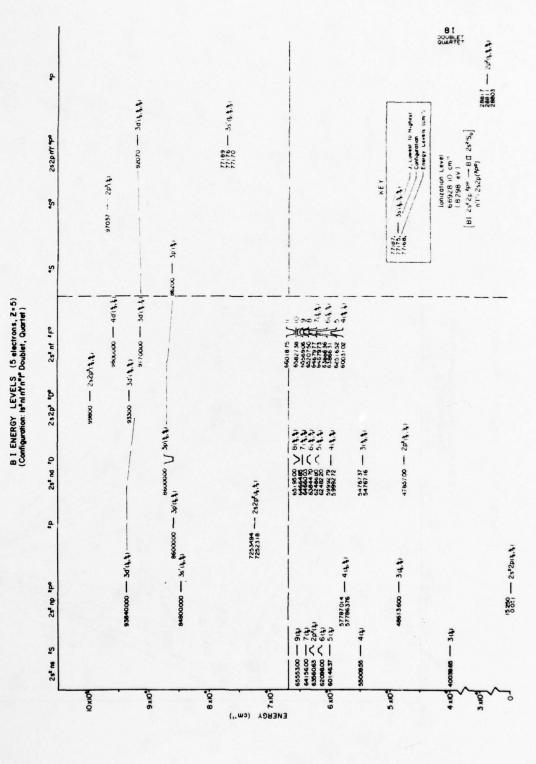
He II ENERGY LEVELS (1 electron, Z=2)
(H I sequence, Configuration: n1)



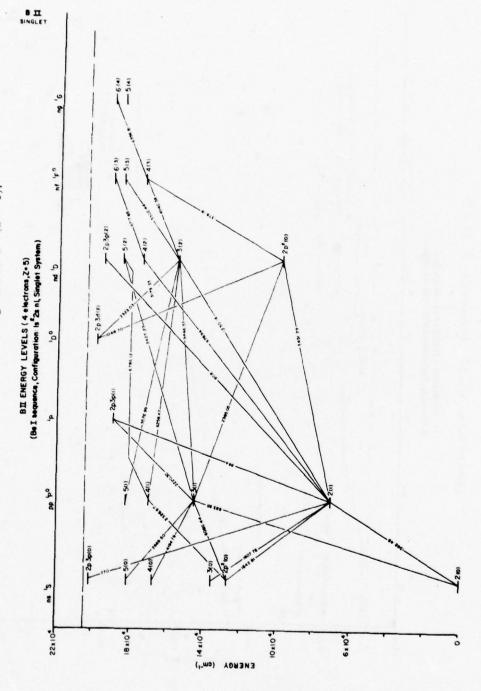
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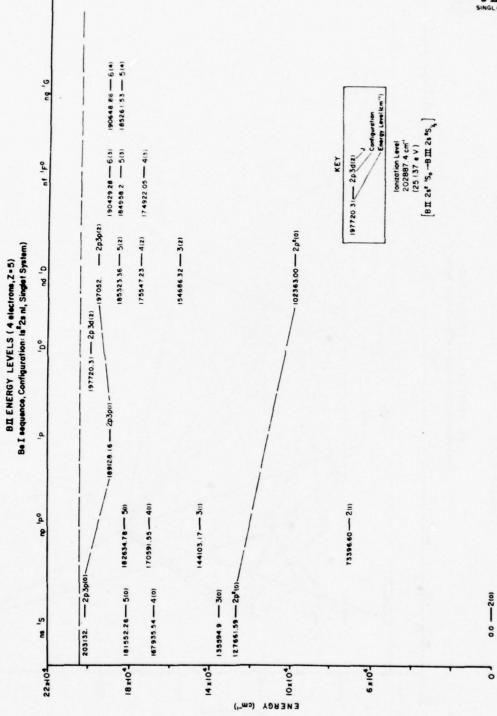
Tabular Data. A-1.13. Diagram for B (Z = 5).



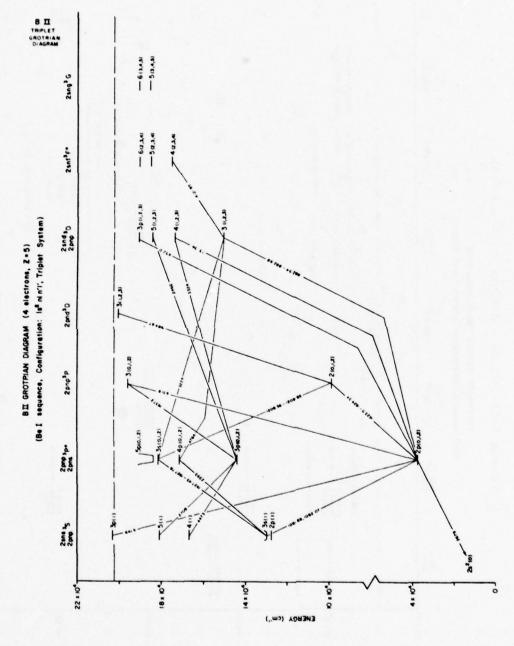
Tabular Data. A-1.14. Diagram for B⁺ (Z = 5).



Tabular Data. A-1.15. Diagram for B^+ (Z = 5).

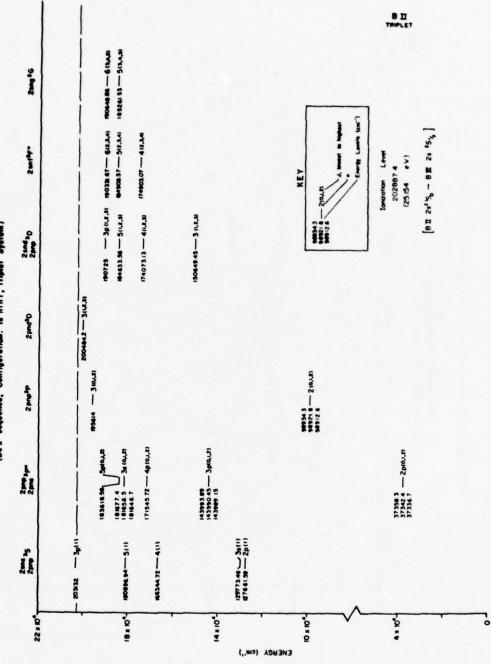


Tabular Data. A-1.16. Diagram for B^+ (Z = 5).

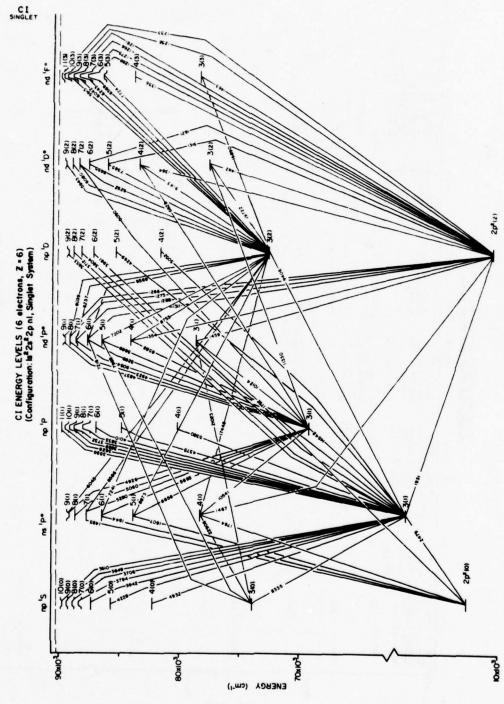


Tabular Data. A-1.17. Diagram for B^+ (Z = 5).

BE ENERGY LEVELS (4 electrons, 2-5) (Be I sequence, Configuration: Ishin'r, Triplet System)

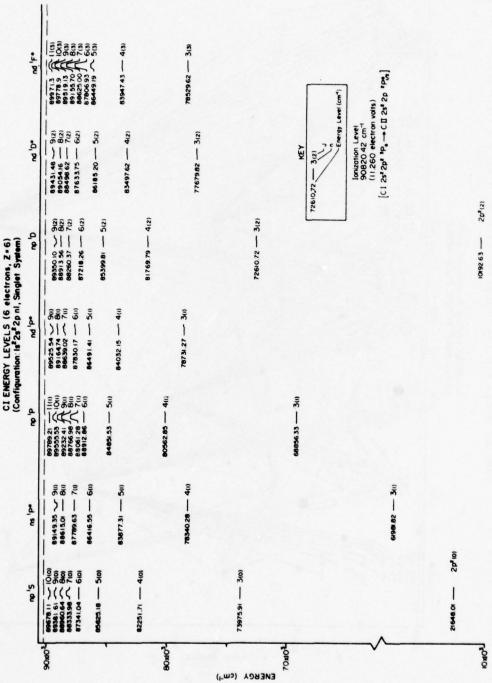




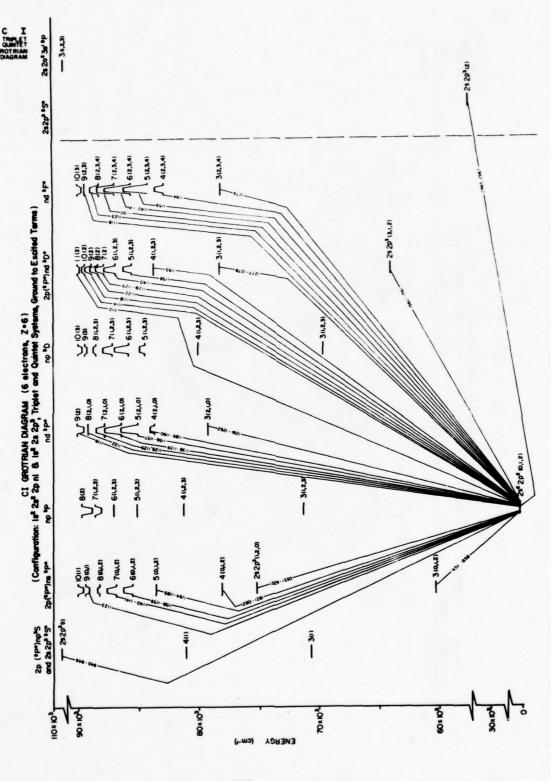


CI

Tabular Data. A-1.19. Diagram for C(Z = 6).

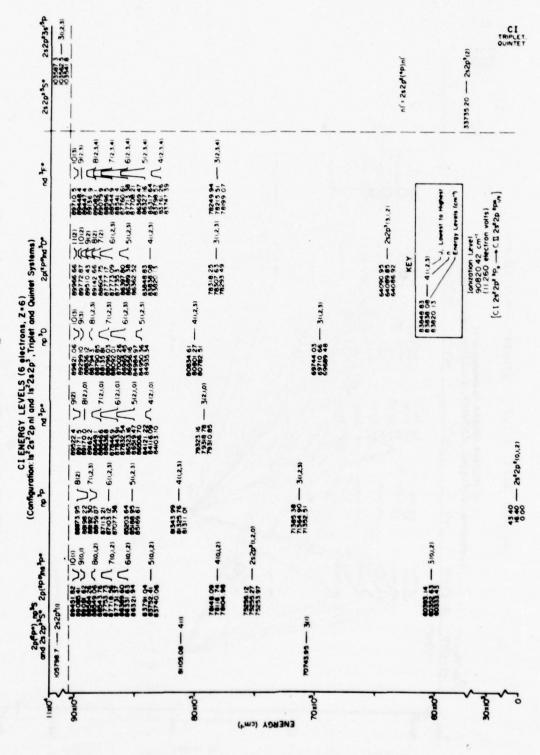


Tabular Data. A-1.20. Diagram for C(Z = 6).



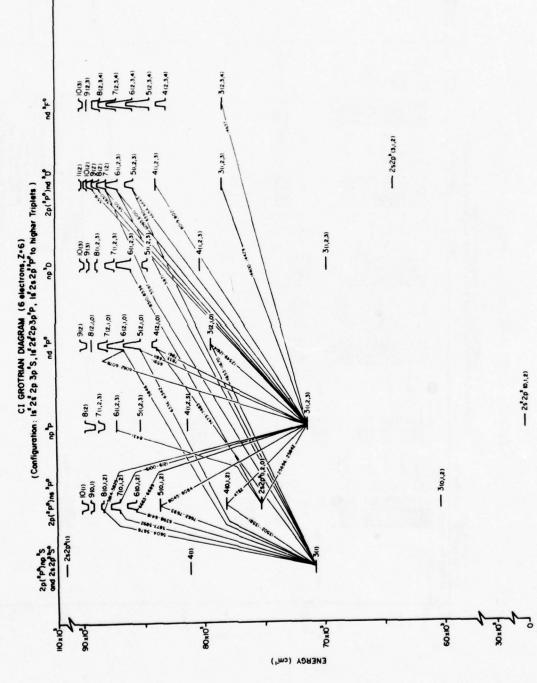
2820 34 P 7 30,2,3) - 2520°(2) 25.20 5 9(2.3) 9(2.3) 7(2.3.4) 5(2,2,4) 1 623,41 . P CI GROTRIAN DIAGRAM (6 electrons, Z=6) (Configuration : $3e^3p^6$, $2s2\beta^3D^6$, $3p^3D$ to higher Triplets, and Quintet to Quintet Terms) Tabular Data. A-1.21. Diagram for C(Z=6). N 50,2,31 2p("P)md "D" 86.23) 7.1.23) 1 60,2,3) 9 - 2\$ 2p (0,1,2) Spr prima to 2p(*P*)np*S and 2s2p*S* - 2x2 p(u) Loxon 90 x 10 -par os 30.00 O 10 ENERGY (cm+)

Tabular Data. A-1.22. Diagram for C (Z = 6).



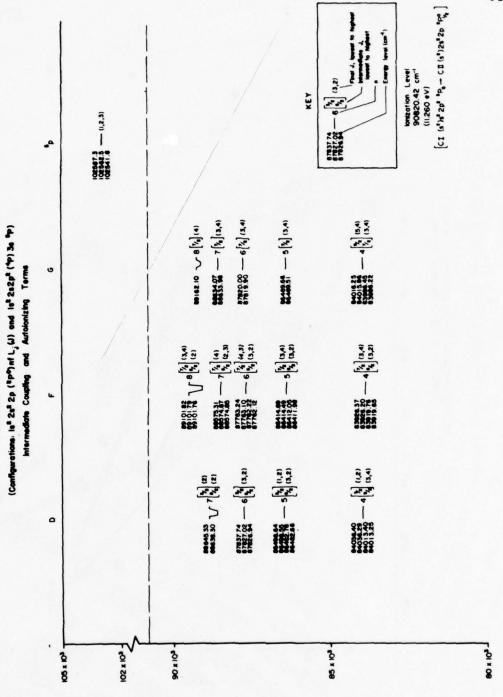
TRIPLET GROTRIAN DIAGHAM



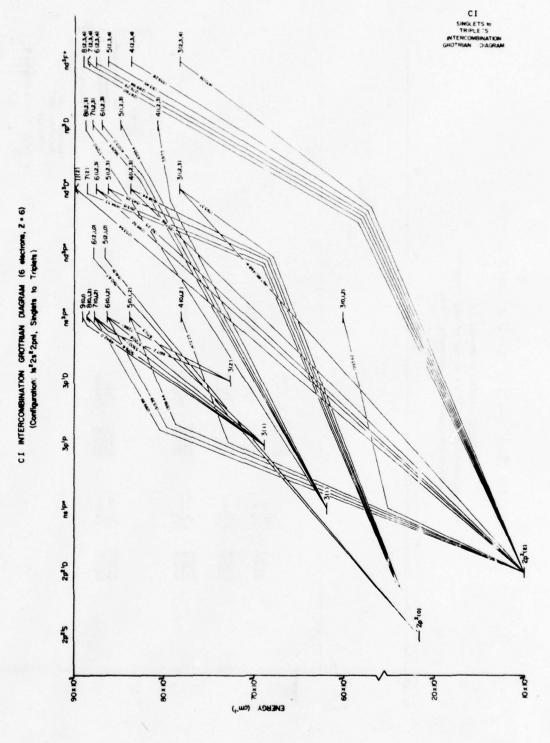


Tabular Data. A-1.24. Diagram for C(Z=6).

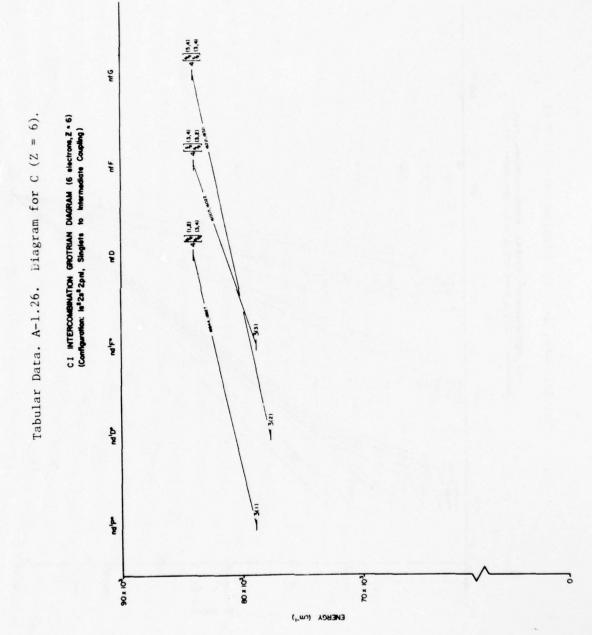
C I ENERGY LEVELS (6 electrons, Z-6)



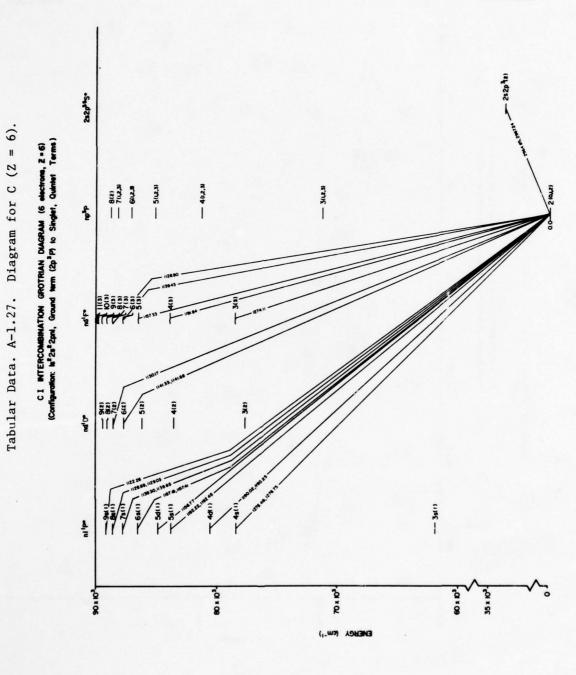
Tabular Data. A-1.25. Diagram for C(Z = 6).



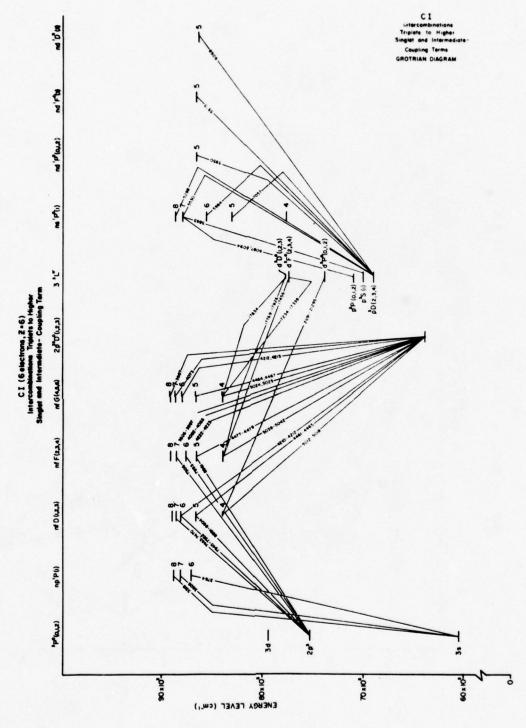
C I
SONGLETS TO
NTERMEDIATE COUPLING
INTERCOMBINATION
GROTRIAN DIAGRAM

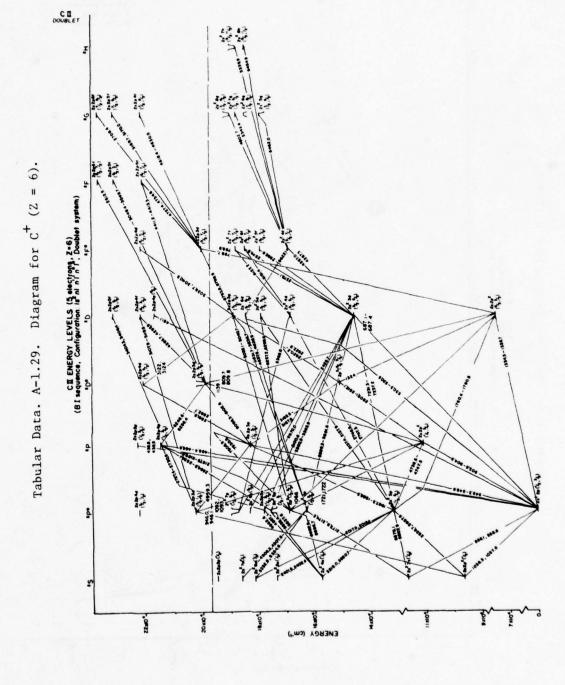


C I
Ground Term (2p P) to
SINGLET, QUINTET
INTERCOMBINATION
GROTRIAN DIAGRAM

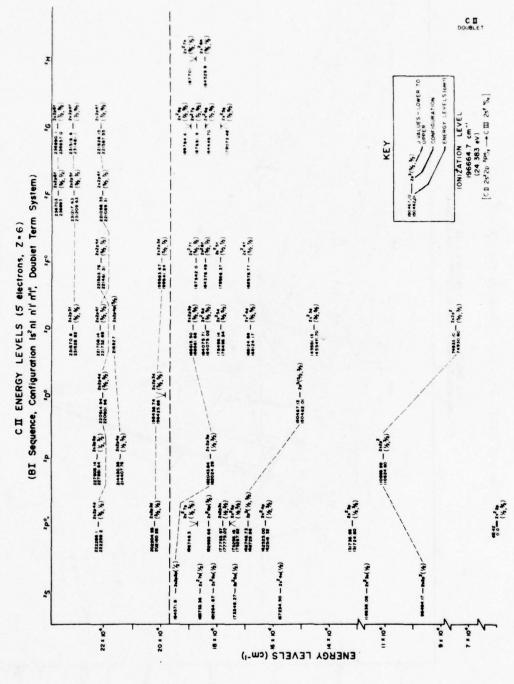


Tabular Data. A-1.28. Diagram for C(Z = 6).

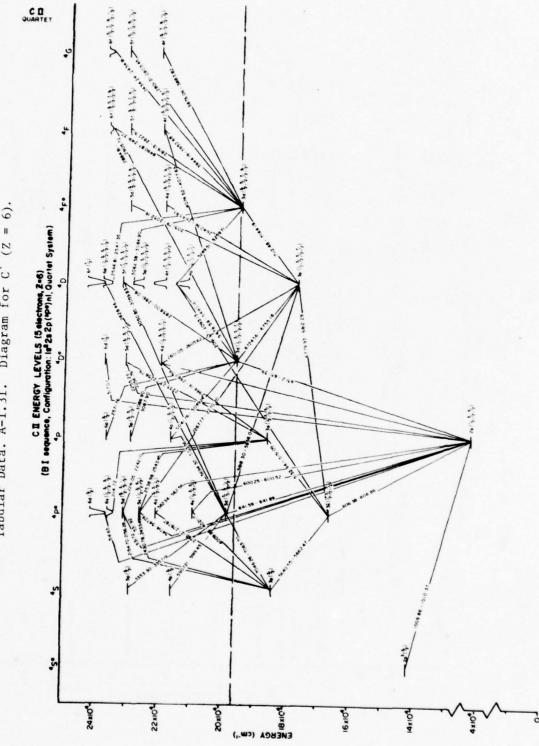




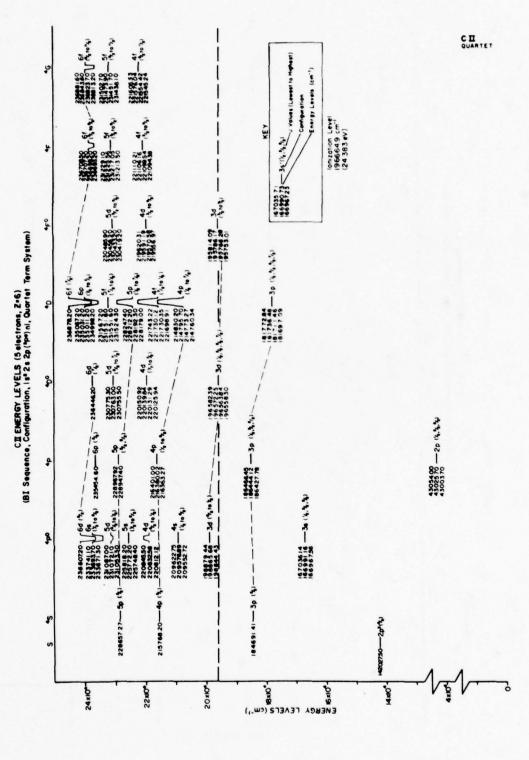
Tabular Data. A-1.30. Diagram for C^+ (Z = 6).



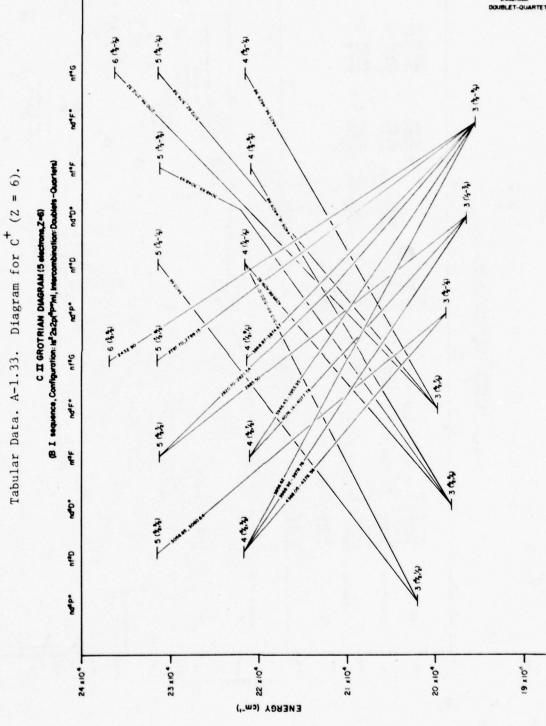
Tabular Data. A-1.31. Diagram for C^+ (Z = 6).

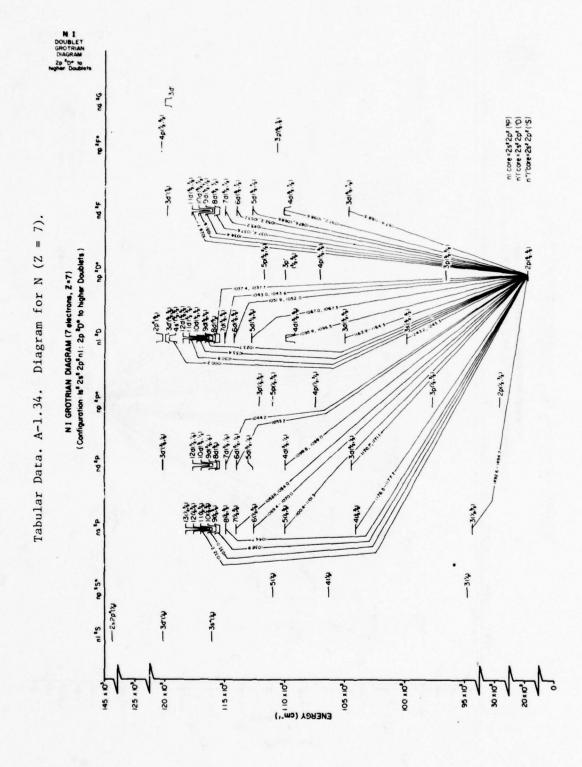


Tabular Data. A-1.32. Diagram for C^+ (Z = 6).



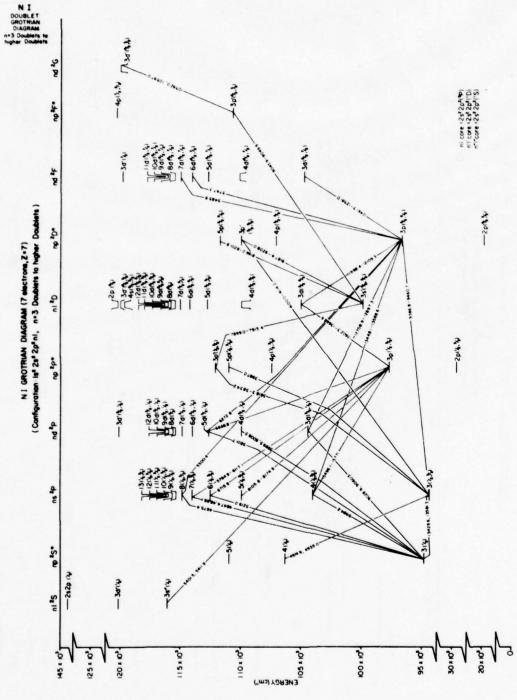
C II INTERCOMBINATION GROTRIAN DIAGRAM DOUBLET-QUARTET



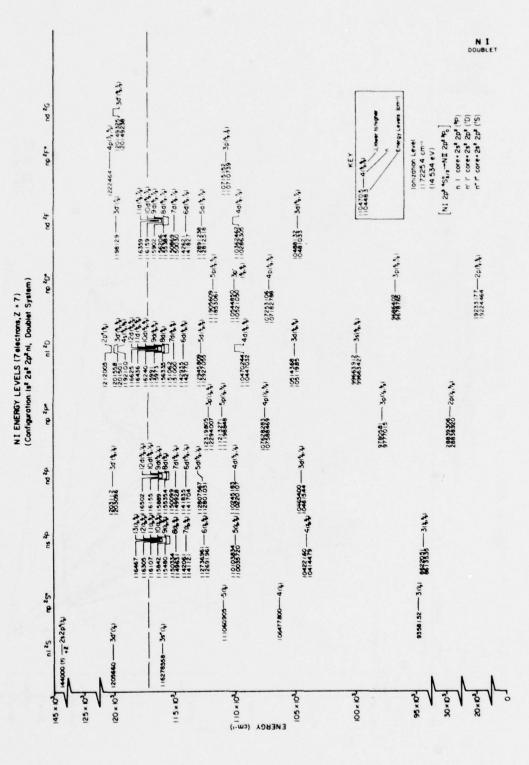


-40(%.%) A36A.W ni core :25, 2pt (PP) n'r core :25, 2pt ('D) n'r core :25, 2pt ('S) - 3pm.1 \$ 60 PE A 404. 20 7 3018.30 Tabular Data. A-1.35. Diagram for N (Z = 7). 3pr. 3) N I GROTRIAN DIAGRAM (7 electrons, 2=7) (Configuration: lss 2s 2ps ni : 2p 2ps to higher Doublets) - Sprt. 4) -2pd.3) A 20. 0.0 -34(4,5) 13/4.4 J 3. 20% -30 S O -2s2p*(%) -30% 138 (1) S I 8 8 8 5 4 5 4 5 4° 145 x 107 100 x 103 115 x 10 125 x 10. 0110 120 = 10 105 x 10

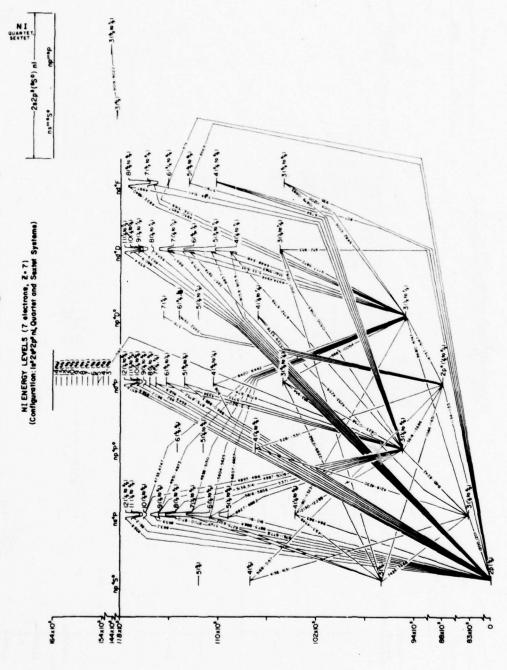




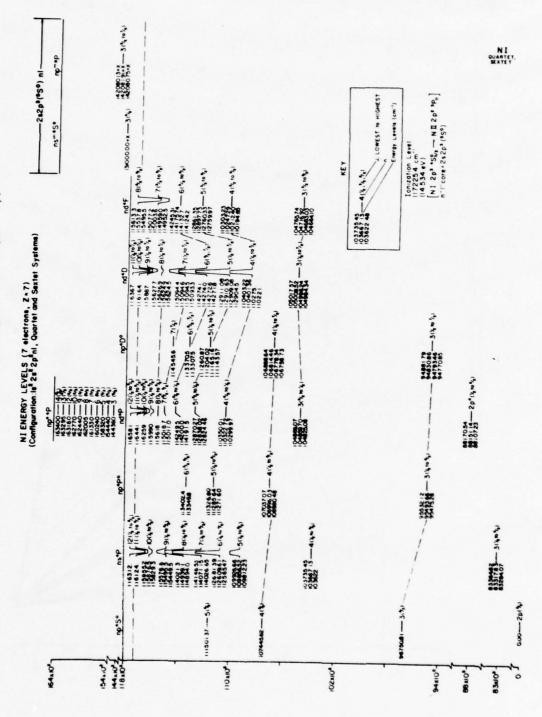
Tabular Data. A-1.37. Diagram for N (Z = 7).



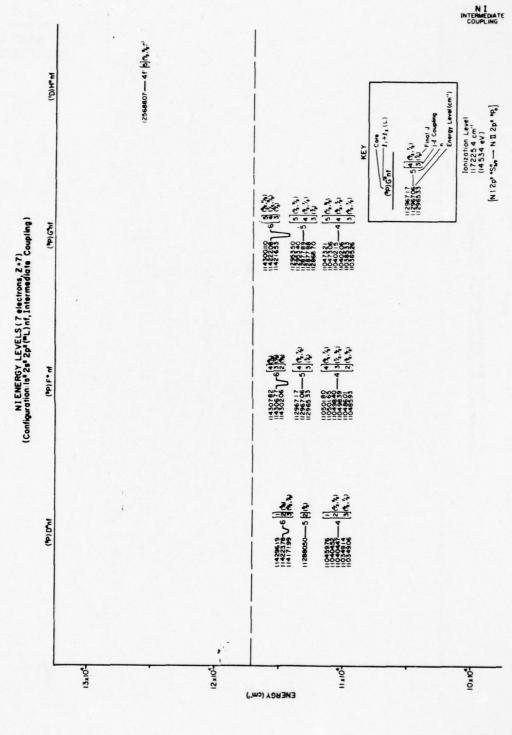
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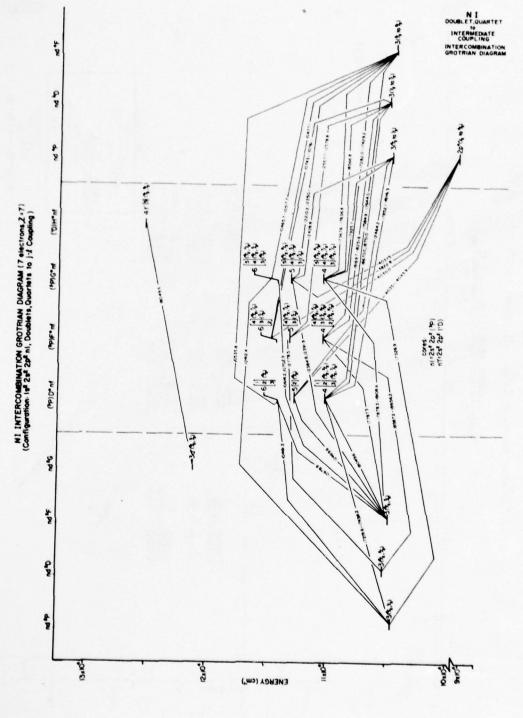
Tabular Data. A-1.39. Diagram for N (Z = 7).



Tabular Data. A-1.40. Diagram for N (Z = 7).

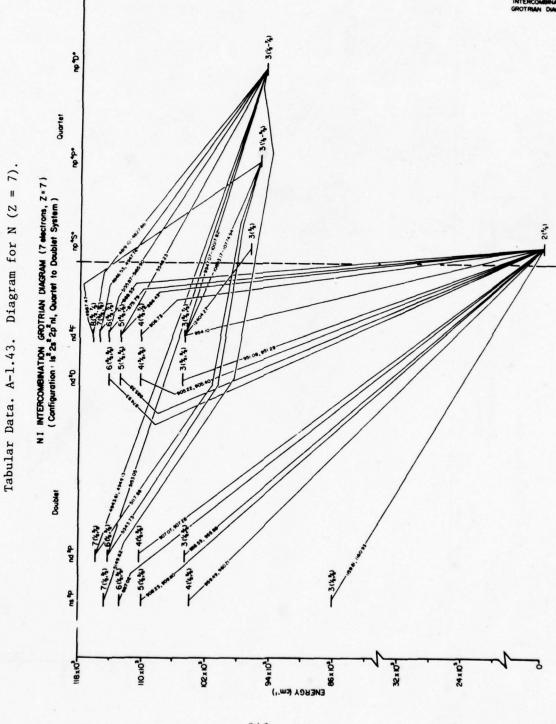


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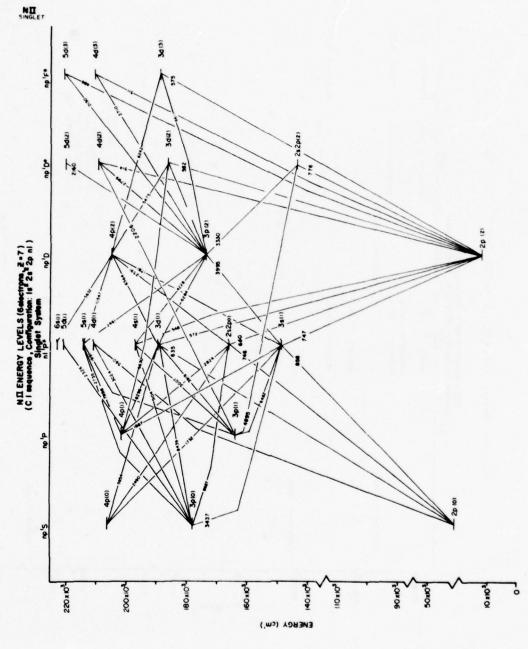


14-19 - 14-19 14-19 - 14-19 15-19 - 14-19 15-19 - 14-19 4-4. 14-15 E - 15-15 7 40-5 Q P0 104-10 664-10 56-10 Quartet Tabular Data. A-1.42. Diagram for N (Z = 7). 3(4-4) N I INTERCOMBNATION GROTRIAN DIAGRAM (7 electrons, 2-7) (Configuration: 1s*2s*2p*nl, Doublet - Quartet Systems) -8288 4 - 82983 no 20. Doublet 8 Sz ou LO 1811 (1-m2) 3210 2410 No xol 102 x 103-20 × 80 ENEBOL

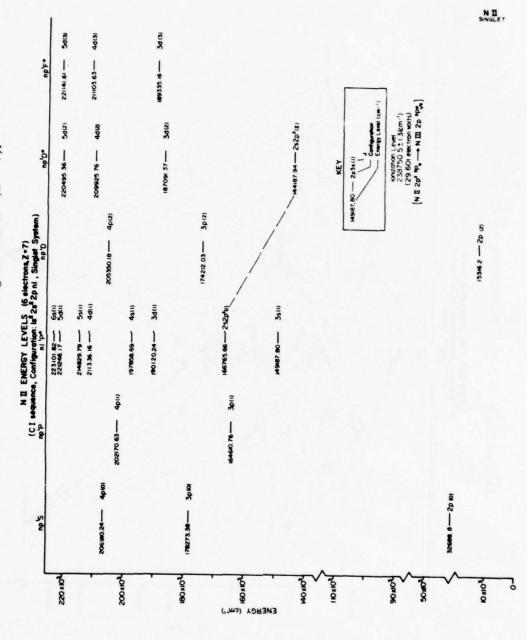
QUARTET TO DOUBLET INTERCOMBINATION GROTRIAN DIAGRAM



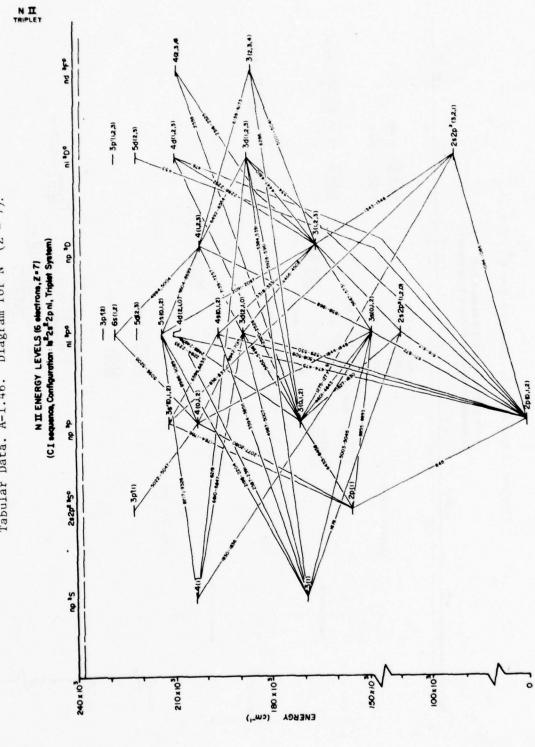
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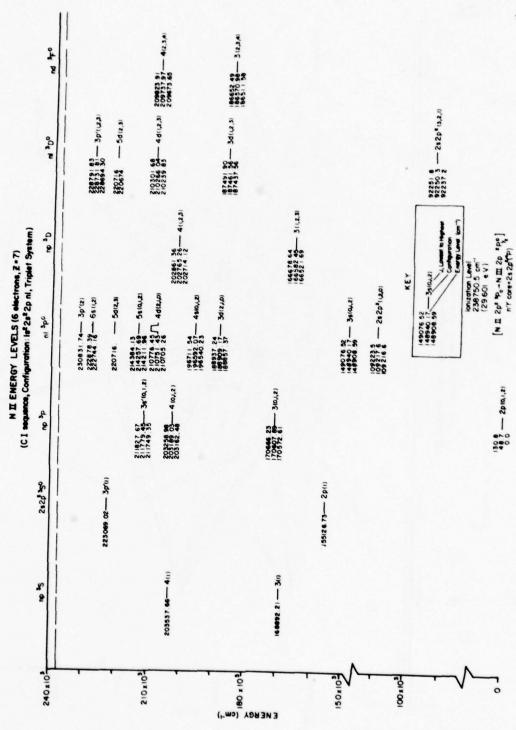
Tabular Data. A-1.45. Diagram for N^+ (Z = 7).

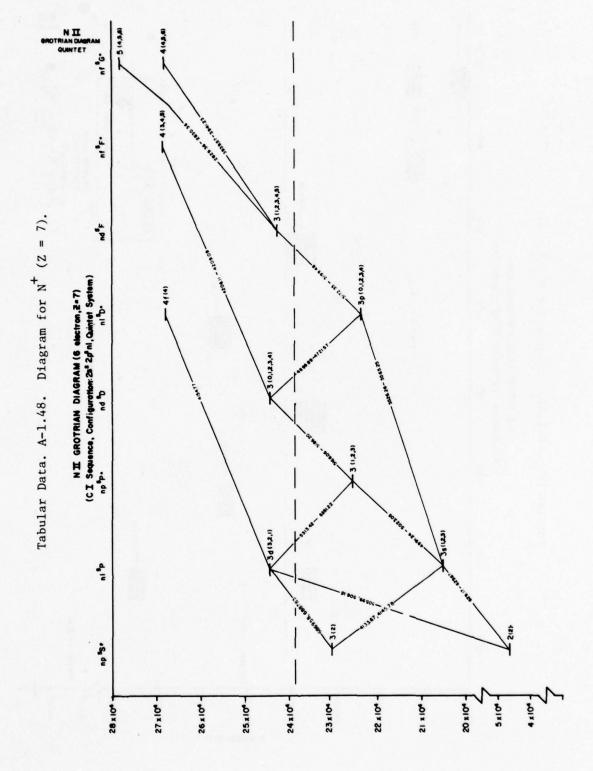


Tabular Data. A-1.46. Diagram for N^+ (Z = 7).

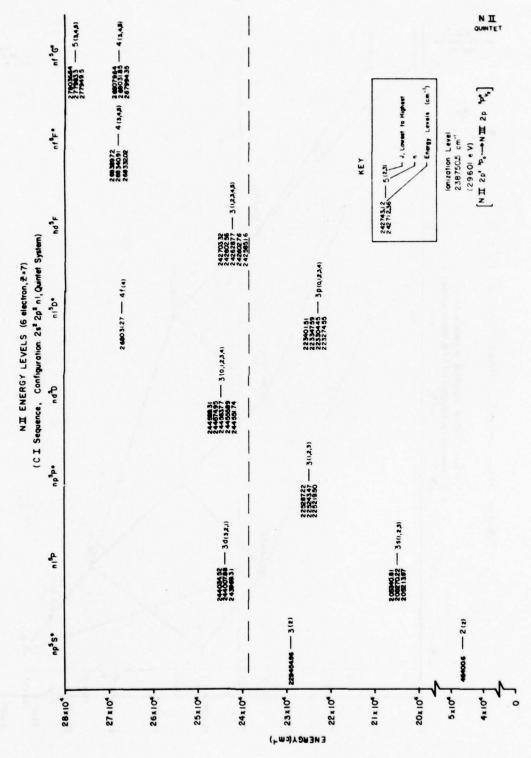


Tabular Data. A-1.47. Diagram for N^+ (Z = 7).

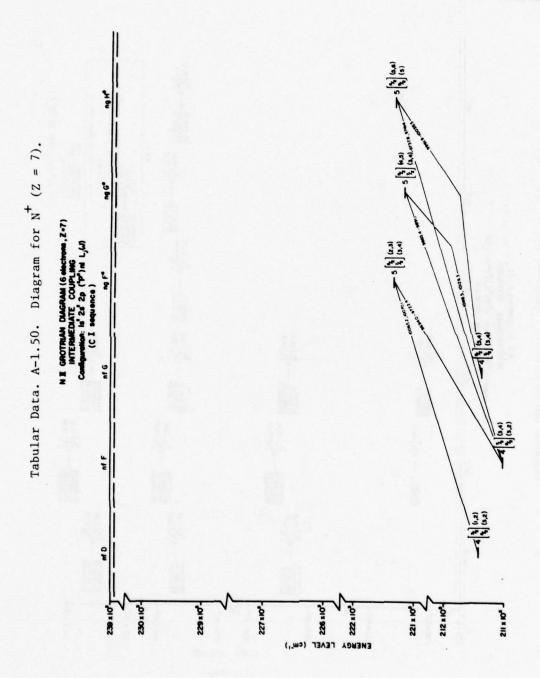


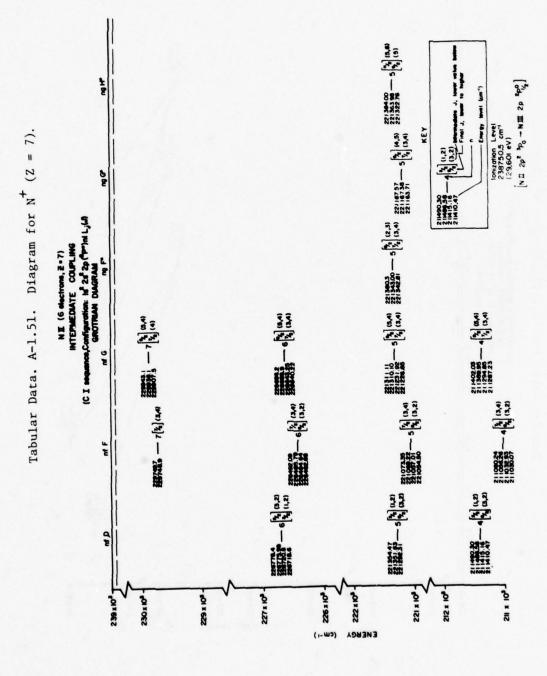


Tabular Data. A-1.49. Diagram for N^+ (Z = 7).



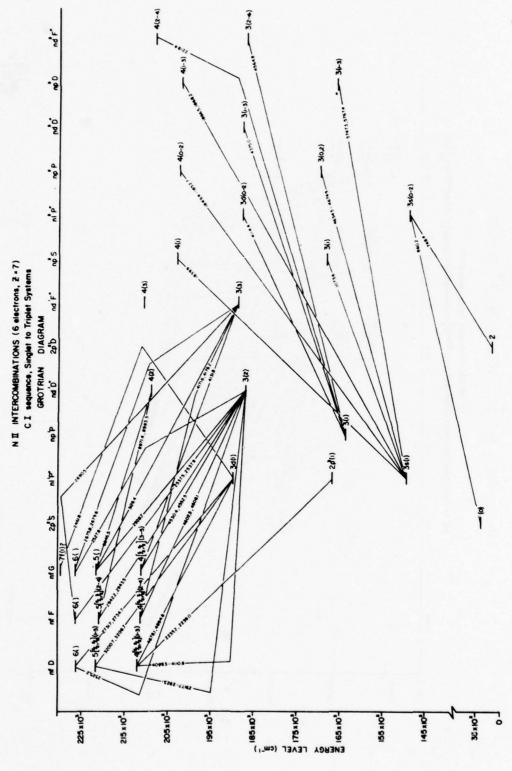
N II NTERMEDIATE COUPLING GROTRIAN DIAGRAM



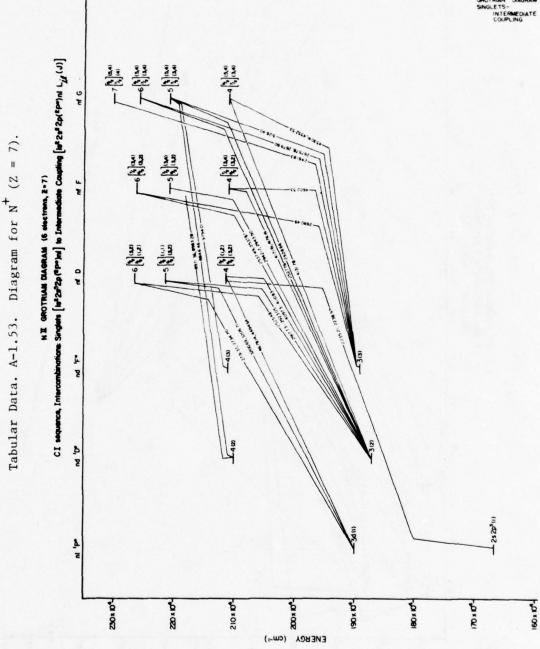


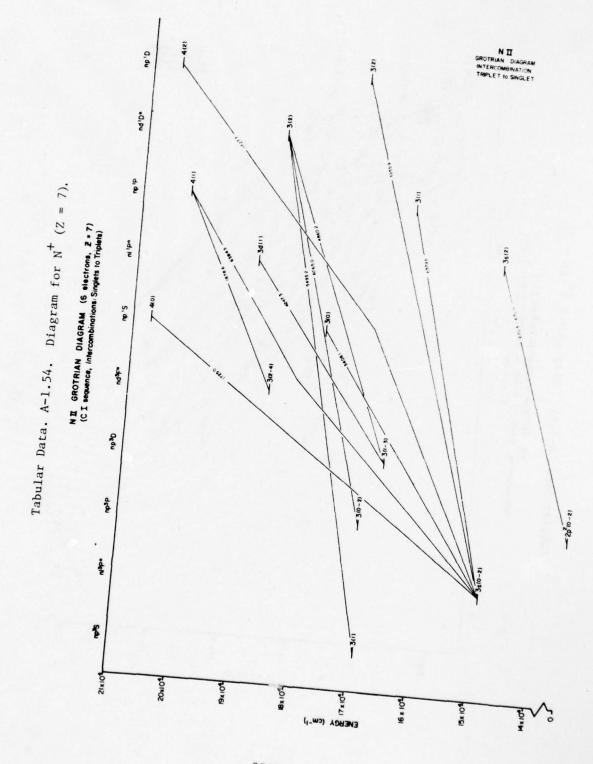
N II NTERCOMBINATIO GROTRIAN DIAGRAM



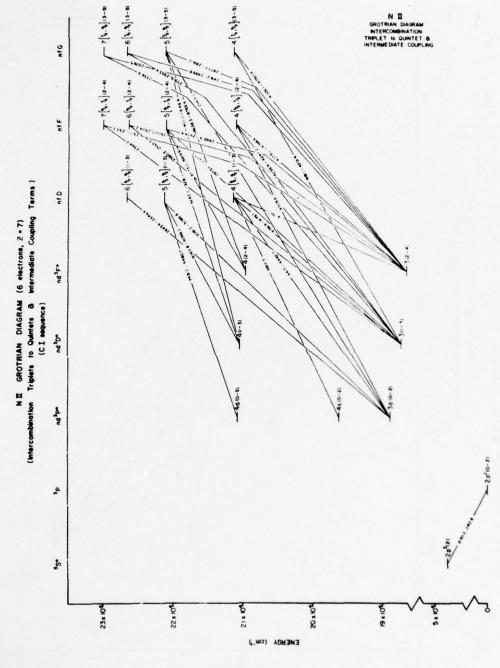




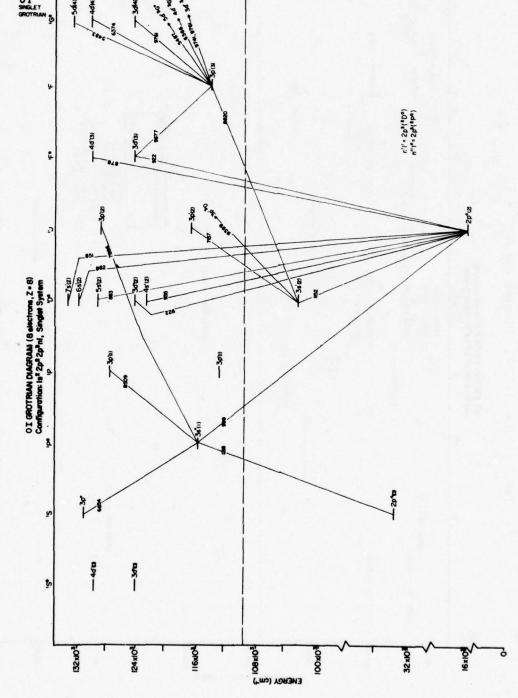




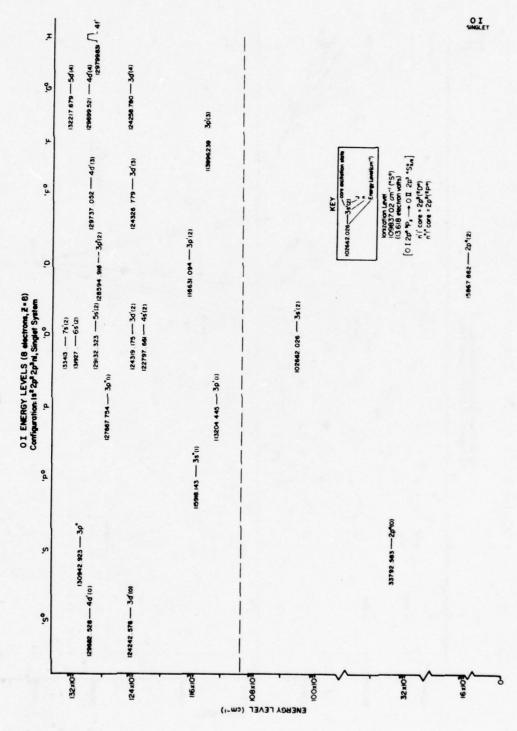
Tabular Data. A-1.55. Diagram for N^+ (Z = 7).



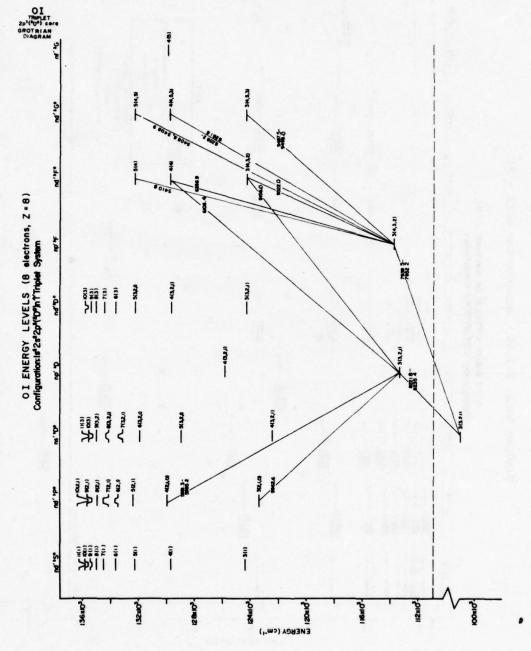
Tabular Data. A-1.56. Diagram for 0 (Z = 8).



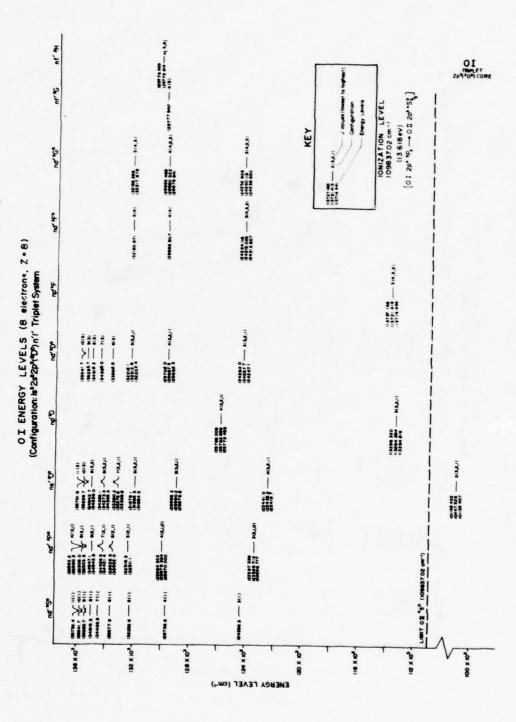
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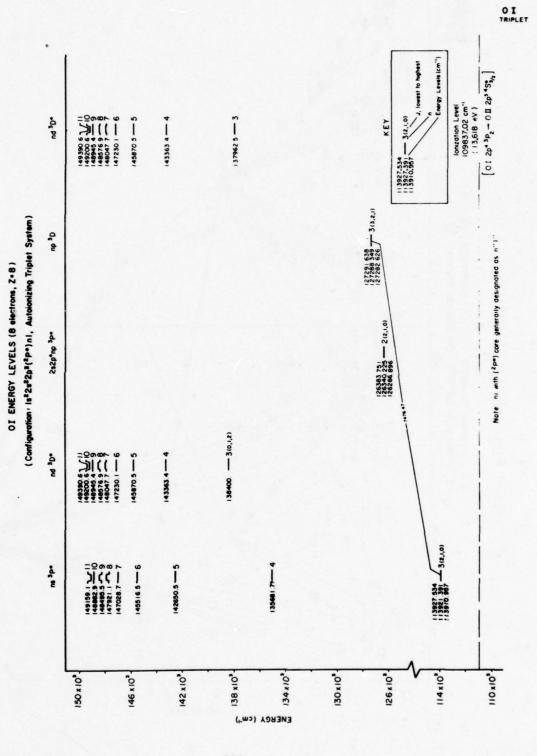
Tabular Data. A-1.58. Diagram for 0 (Z = 8).



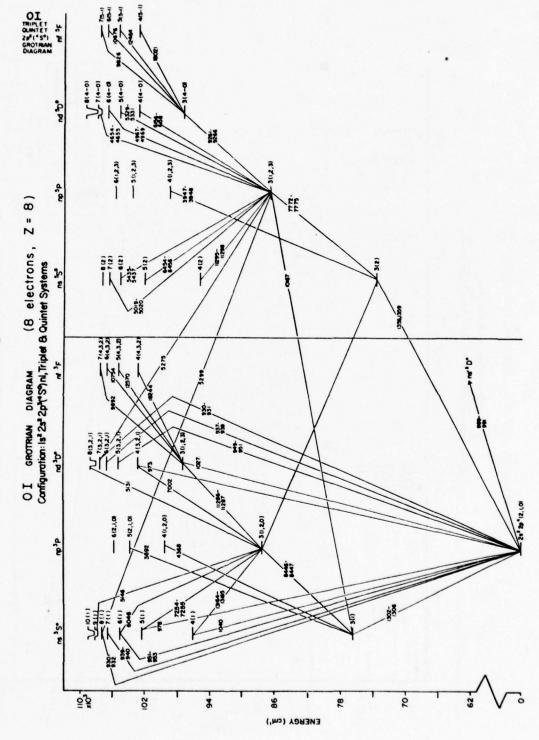
Tabular Data. A-1.59. Diagram for 0 (Z = 8).



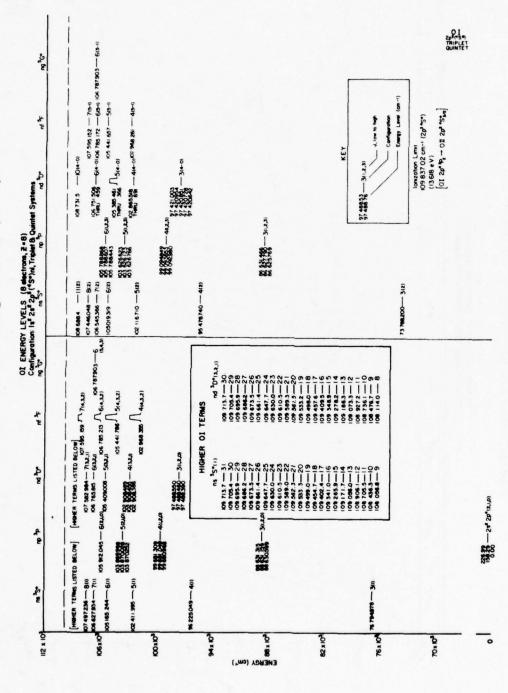
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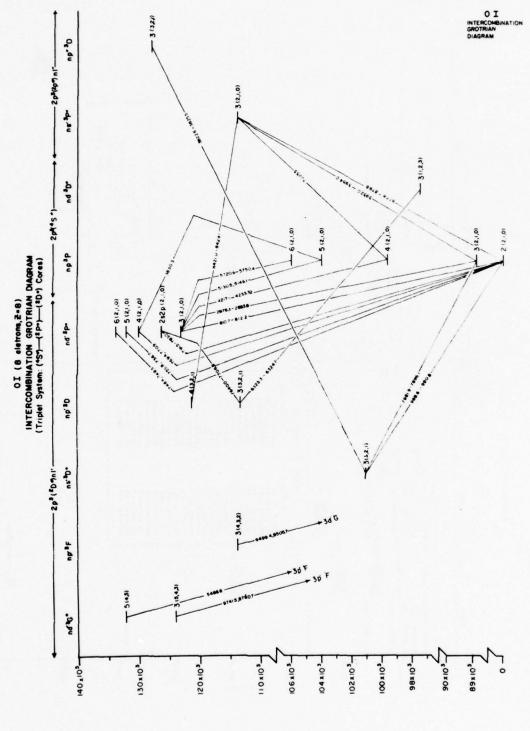
Tabular Data. A-1.61. Diagram for 0 (Z = 8).



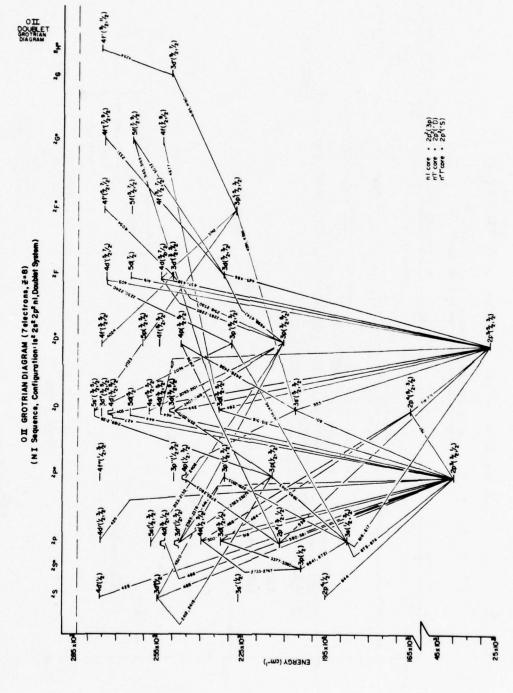
Tabular Data. A-1.62. Diagram for 0 (Z = 8).



Tabular Data. A-1.63. Diagram for 0 (Z = 8).



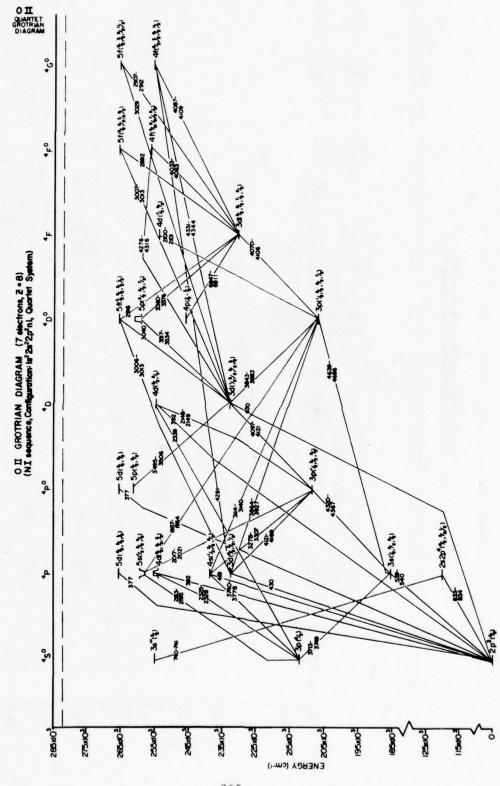
Tabular Data. A-1.64. Diagram for 0^+ (Z = 8).



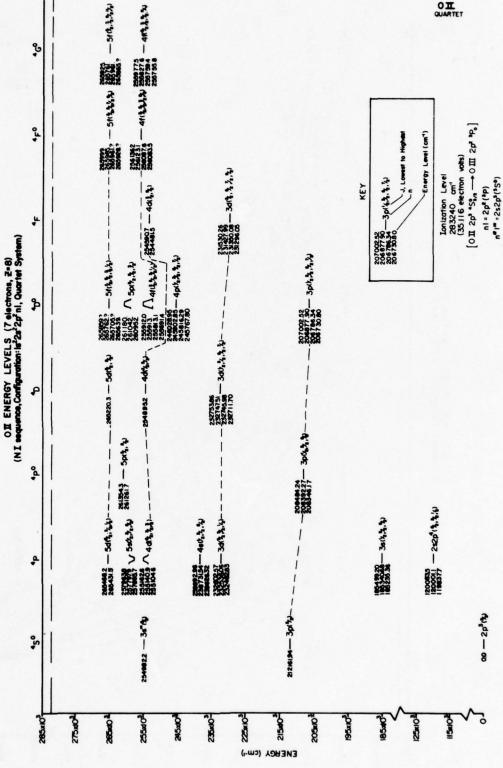
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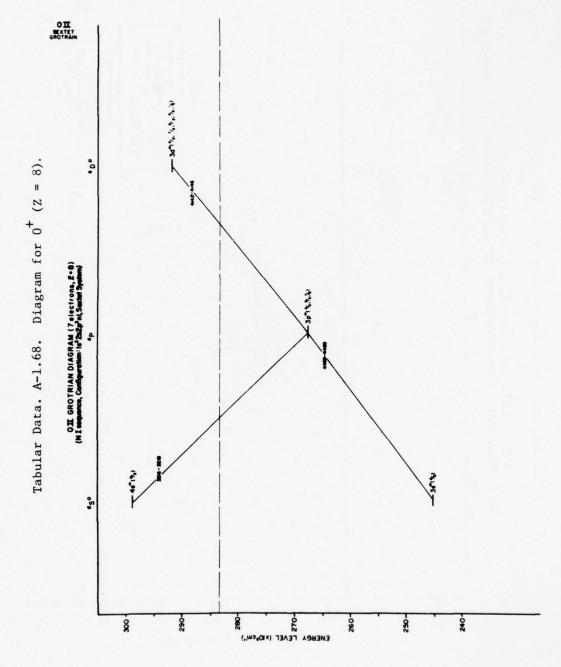
2761091 - 44 (9,1/2) OII 200524~34(½) 200525~4*(½) 200525~4*(½) 200 ÷. 9 2738973-44(1/2)-2736112-44(1/2/2) 27820-41(1/2/2) 273801-34(1/2/2) 278063-41(1/2/2) 274722-41(1/2/2) 2738786-41(1/2/2) 2738413-41(1/2/2) $-260578! -54(7_2) \frac{265999}{260968!} -5!(\frac{3}{2}7_2) \frac{369992}{2601650} -5!(\frac{3}{2}7_2)$ - Core Excitation State n) care: 2p/36)
n'(care: 2p/36)
n'(care: 2p/36)
[I 2p³ *5₂₇ • 0 II 2p² *b₀] .5° -Energy Level Ionization Level 283240 cm⁻¹ (3516eV) 206972 3 - 34 (9, 3,) 2004000 - 34 なん (2005) - 36 (なん) - 1 - 1 - 225 203 35 - 34 (なん) - 1 - 1 - 225 203 35 - 34 (なん) - 25 10 (なん) KEY £. OIL ENERGY LEVELS (7 electrons, 2=8) (NI Sequence, Configuration: 1s² 2s² 2p² ni, Doublet System) 2 21152196 34 3,5/1 -26938 4-2019, 1,1 0 265656 — 54(½) — — 8863-3*(%,%) 1659960 -20 (3,3/2) 0, 404669 - 203(3,1/2)-. \$\$\$\$ 40(4.%) (4.4) 化一层 4 20304221-36(4) .S. 220001. -34(1/2) 1957104-2014 S 285x10 256x 10-225x10 195 x 102 25 x 104 **2**0×38 45 xIO3 ENERGY (cm-1)

Tabular Data. A-1.66. Diagram for 0^+ (Z = 8).

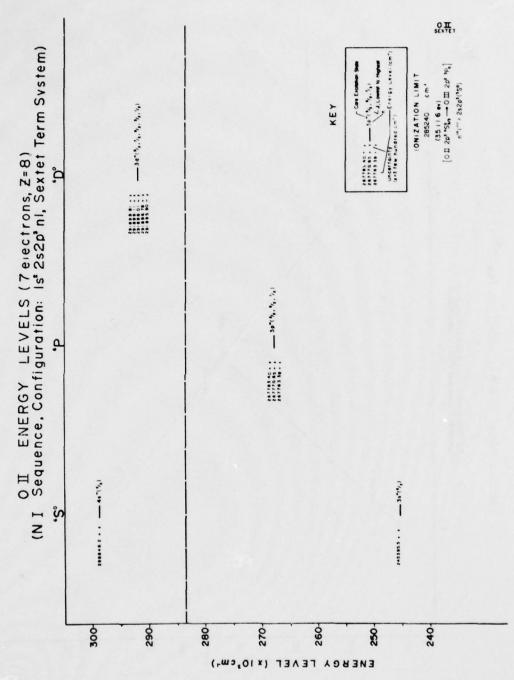


Tabular Data. A-1.67. Diagram for 0^+ (Z = 8).



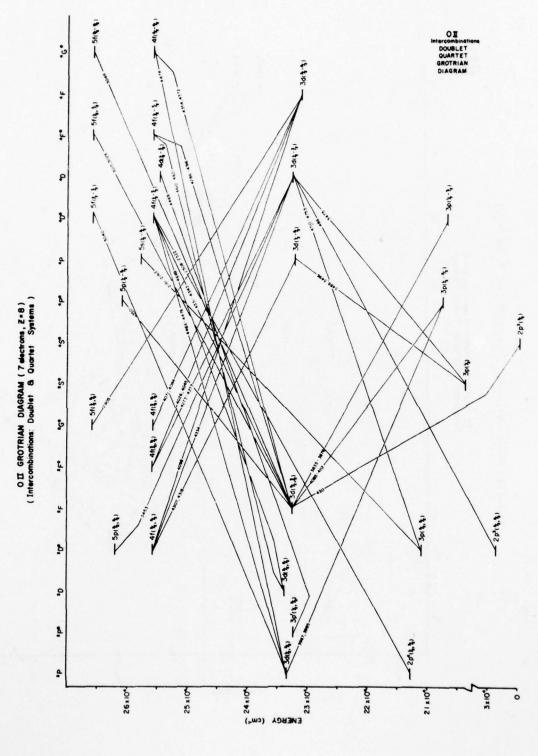


Tabular Data. A-1.69. Diagram for 0^+ (Z = 8).

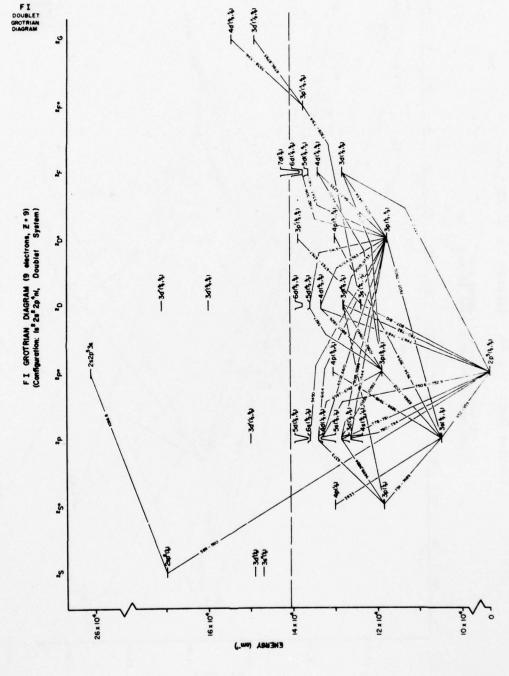


1.

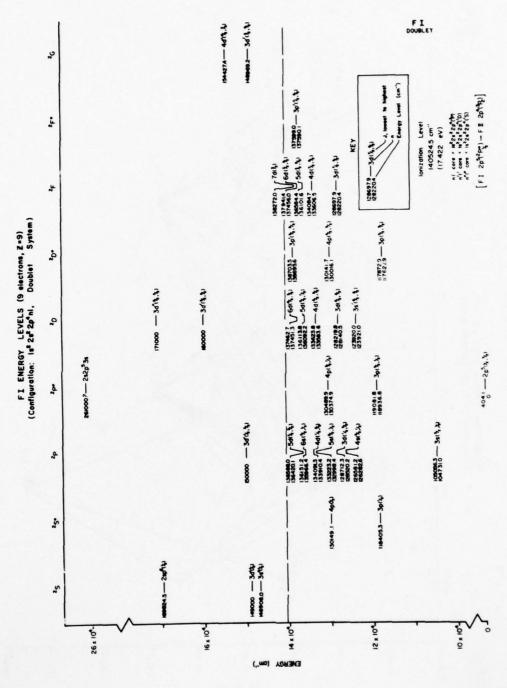
Tabular Data. A-1.70. Diagram for 0^+ (Z = 8).



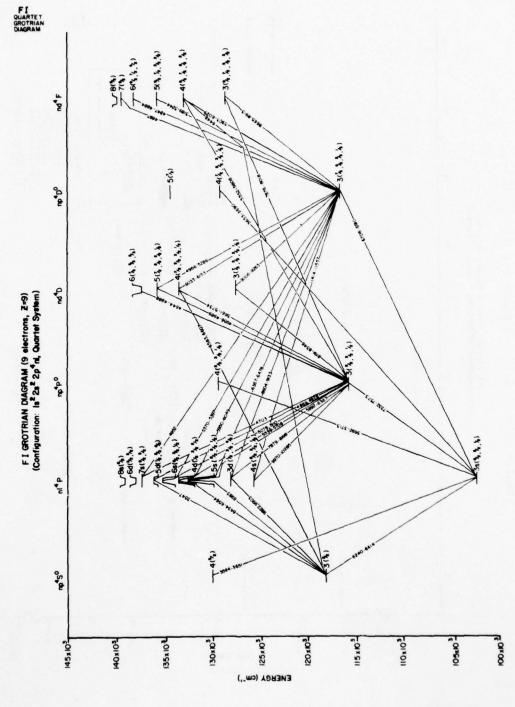
Tabular Data. A-1.71. Diagram for F (Z = 9).



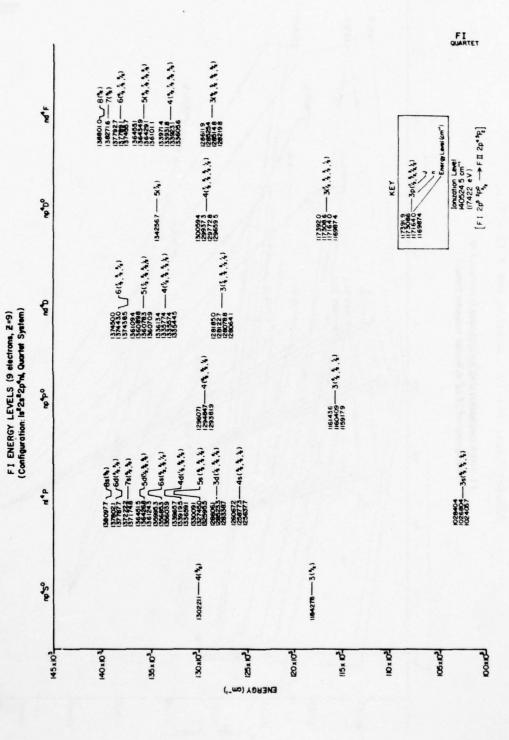
Tabular Data. A-1.72. Diagram for F(Z = 9).



Tabular Data. A-1.73. Diagram for F (Z = 9).

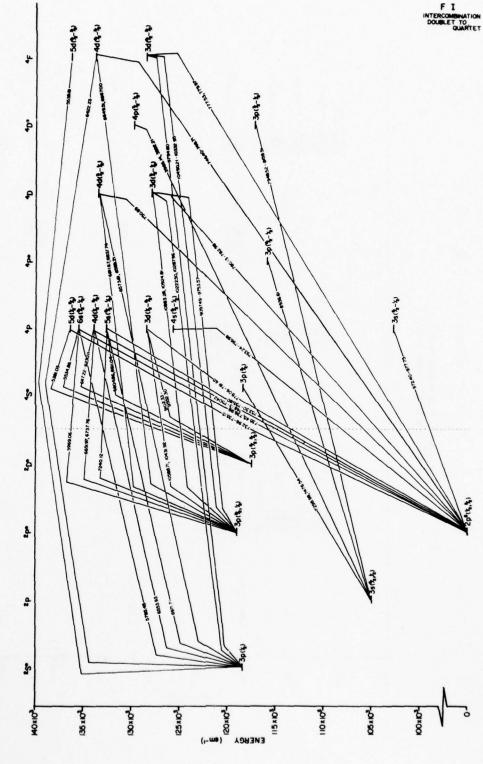


Tabular Data. A-1.74. Diagram for F (Z = 9).

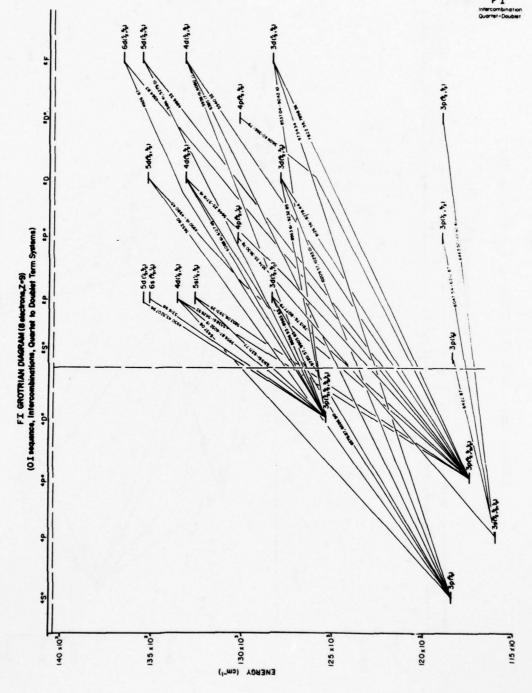


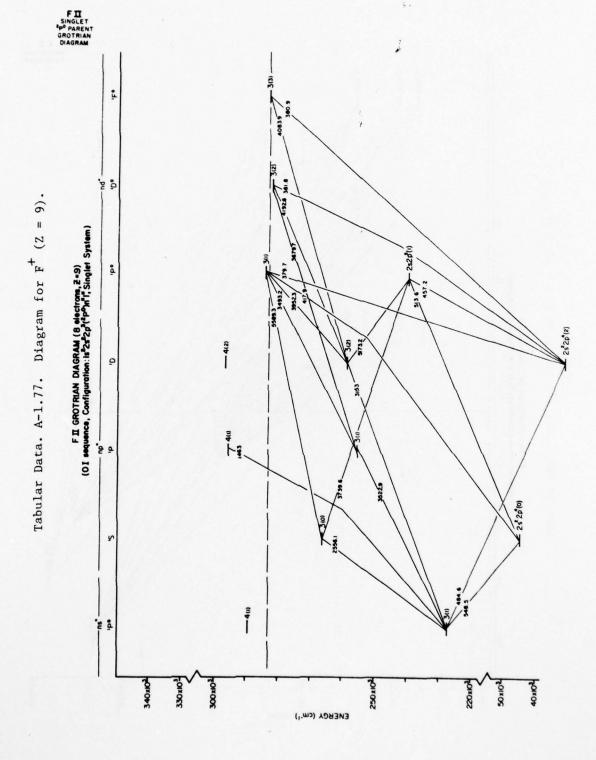
Tabular Data. A-1.75. Diagram for F(Z = 9).

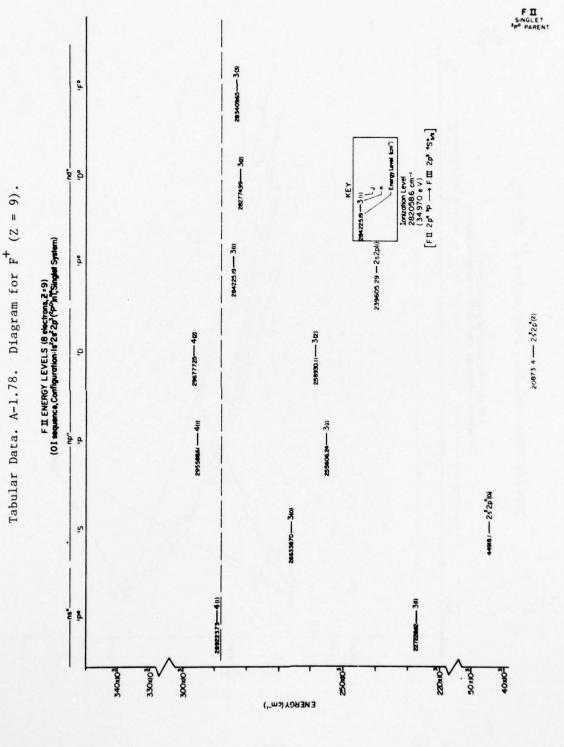
F.I. INTERCOMBINATION GROTRIAN DIAGRAM (9 electrons, Z=9) Configuration: Is 2s 2p n, Doublet to Quarter System



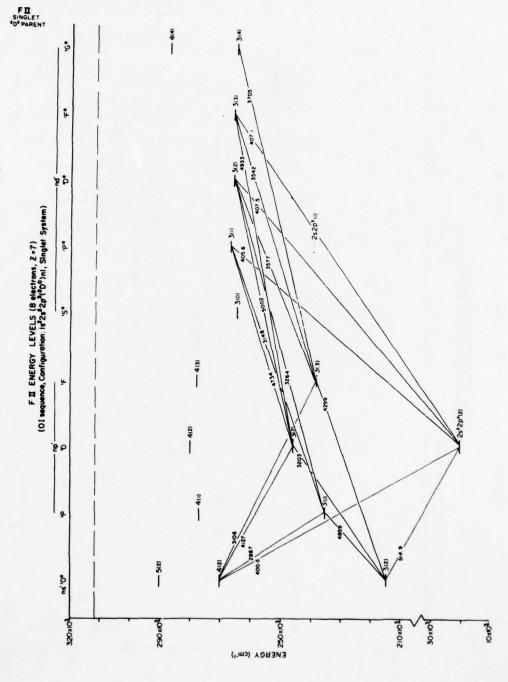




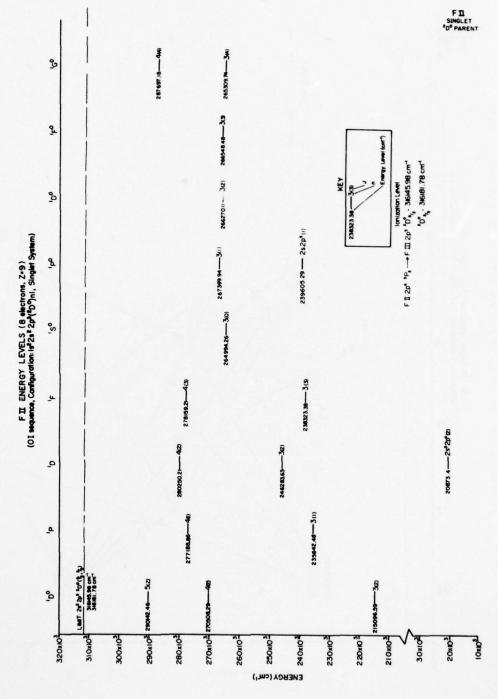




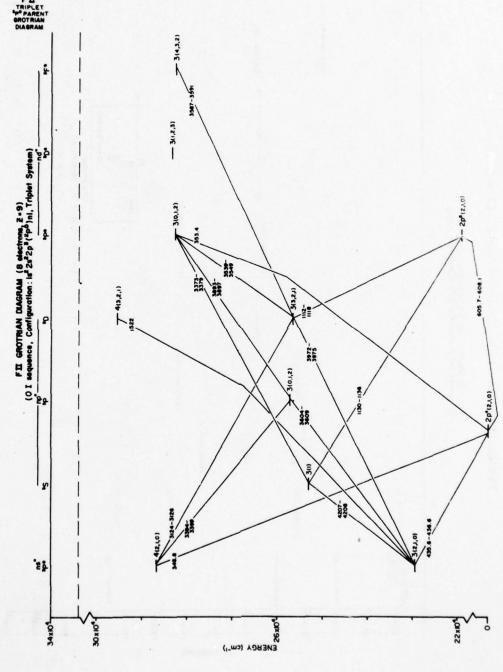
Tabular Data. A-1.79. Diagram for F^+ (Z = 9).



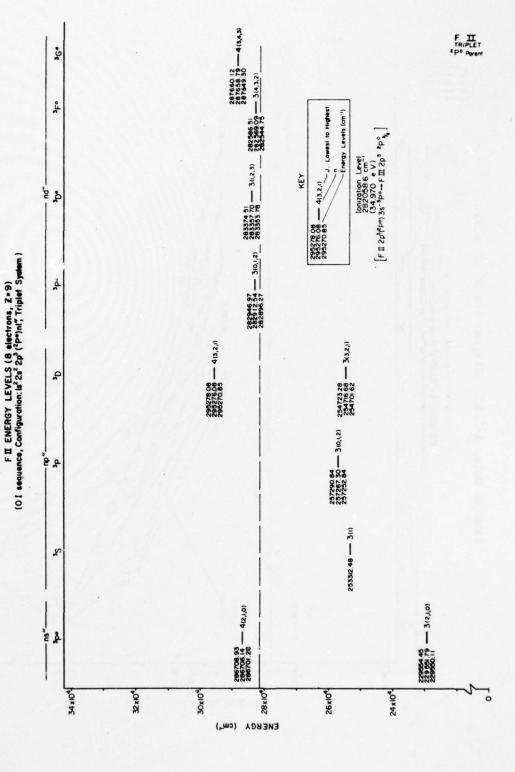
Tabular Data. A-1.80. Diagram for F^+ (Z = 9).

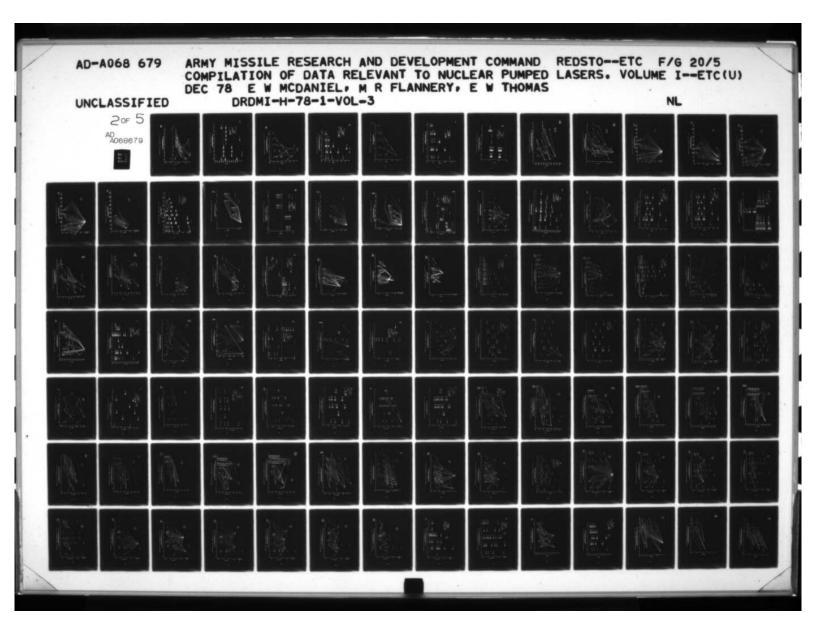


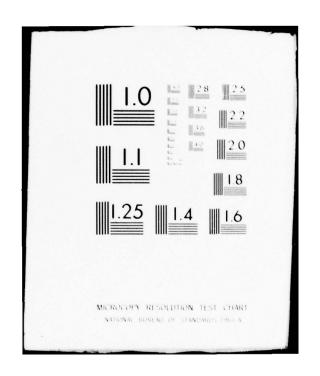
Tabular Data. A-1.81. Diagram for F^+ (Z = 9).



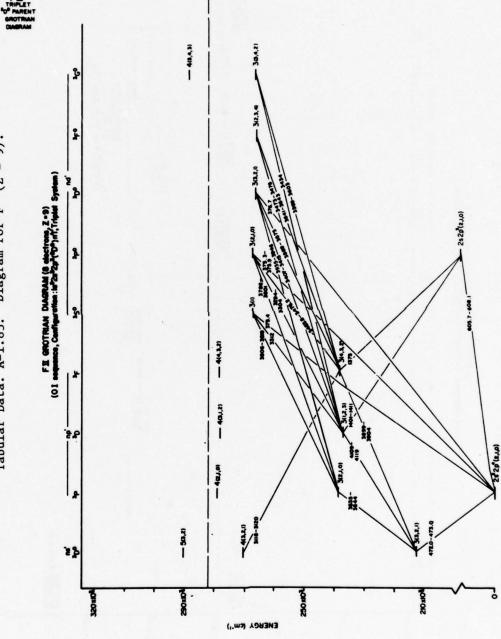
Tabular Data. A-1.82. Diagram for F^+ (Z = 9).



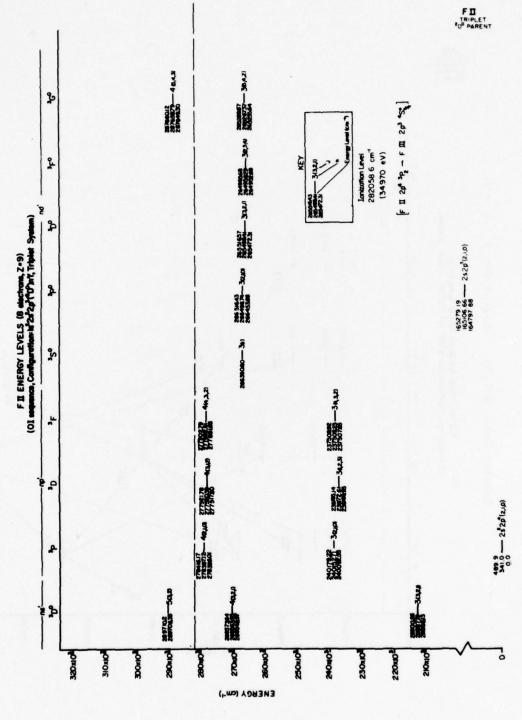




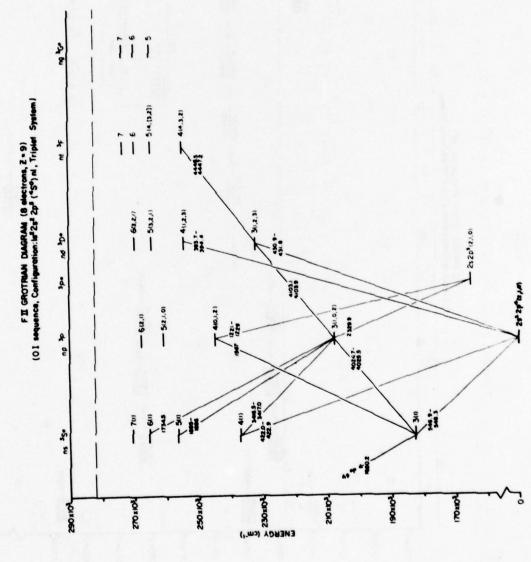




Tabular Data. A-1.84. Diagram for F^+ (Z = 9).

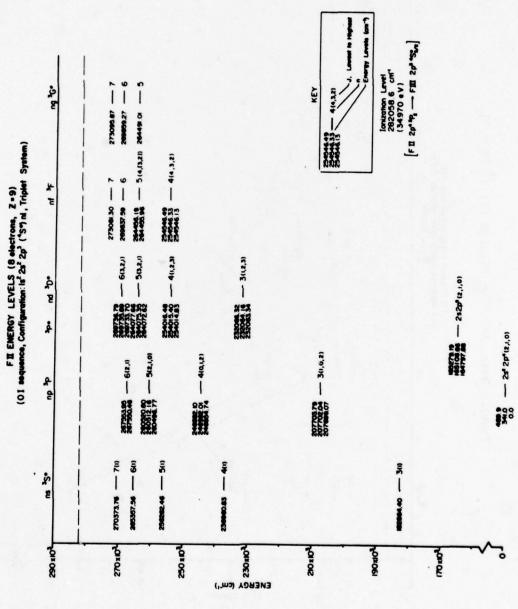


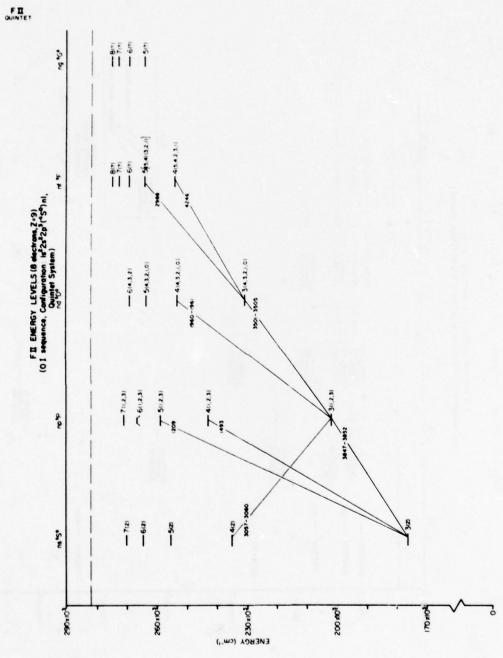
Tabular Data. A-1.85. Diagram for F^+ (Z = 9).



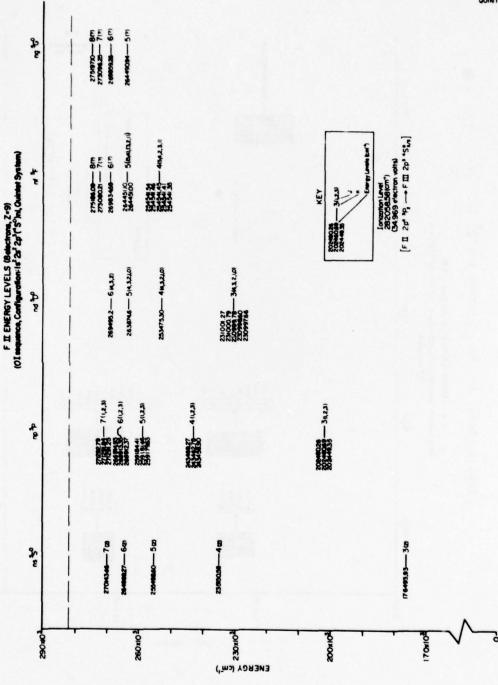




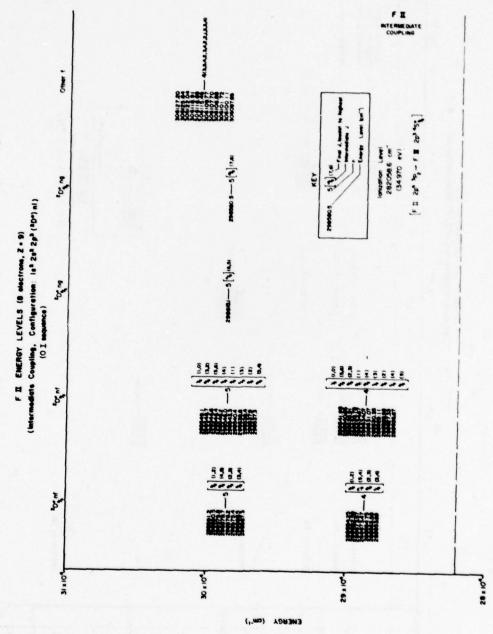


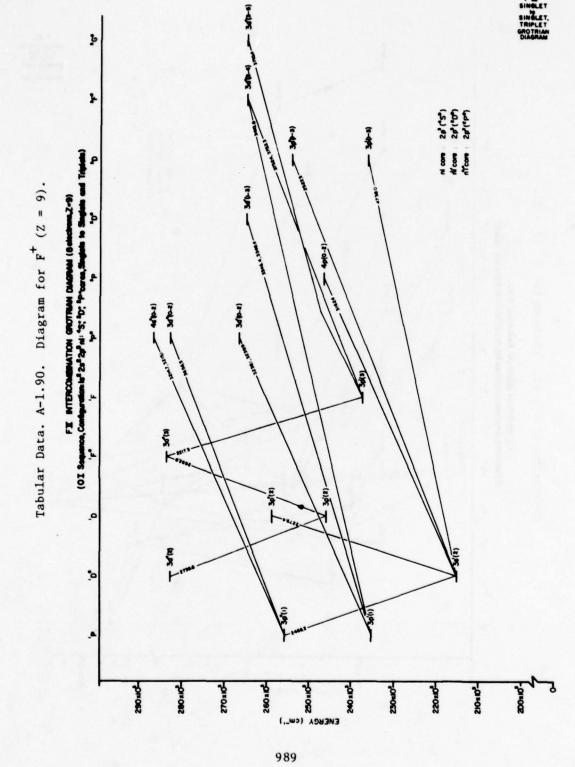


Tabular Data. A-1.88. Diagram for F^+ (Z = 9).



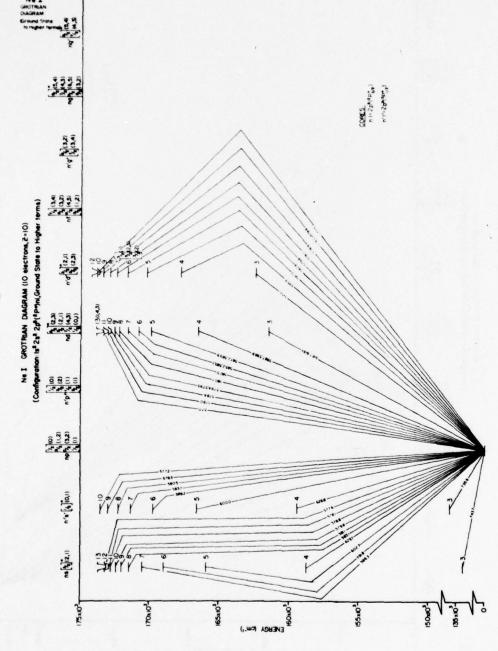
Tabular Data. A-1.89. Diagram for F^+ (Z = 9).



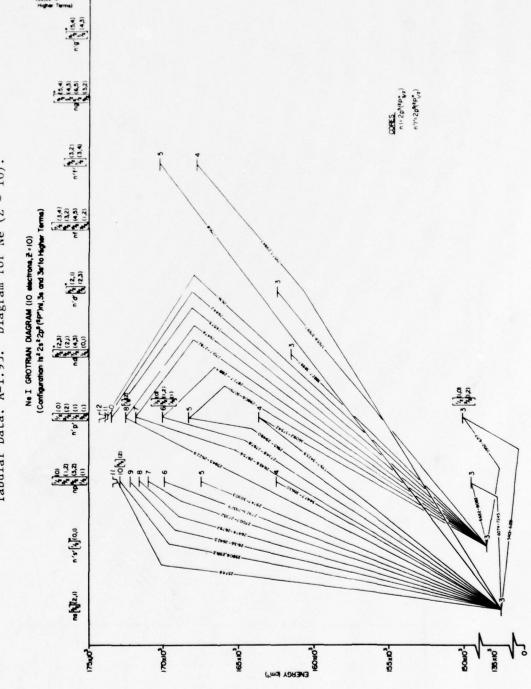


. u nd core : 20 (15") nT' core : 20" (10") n" " core : 20" (10") . Tabular Data. A-1.91. Diagram for F^+ (Z = 9). F.E. GROTRIAN DIAGRAM (8 olectrons, 2-9)
(OI sequence, intercombination; Oxiginal, Triples Terms to Singles & Triples) ٥ 30 S S 29 x 10 T 16.5 x 10 % 26 a 10-23x10* ENERGY (cm.)

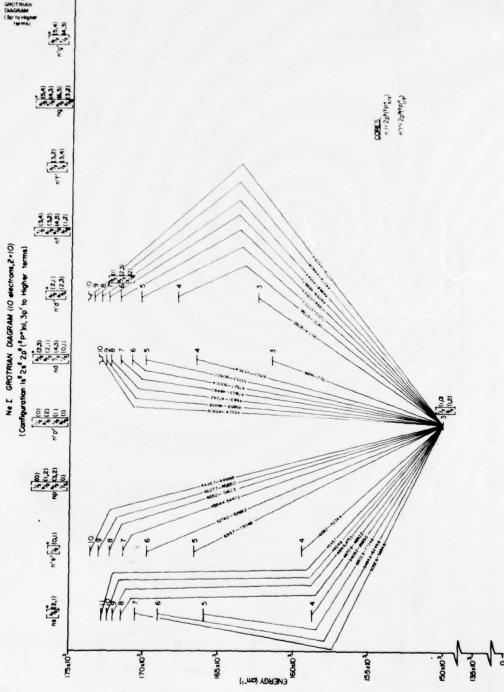
Tabular Data. A-1.92. Diagram for Ne (Z = 10).



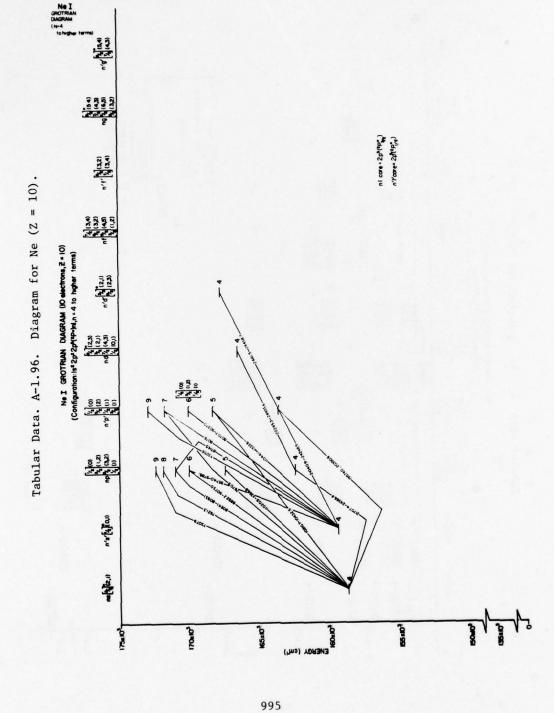
Tabular Data. A-1.93. Diagram for Ne (Z = 10).



CALL STAN Tabular Data. A-1.94. Diagram for Ne (Z = 10). (10)[4],0,0 ns[4]2,!)

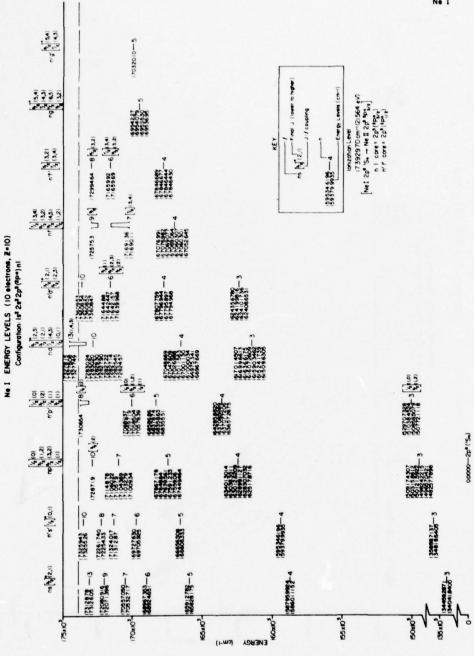


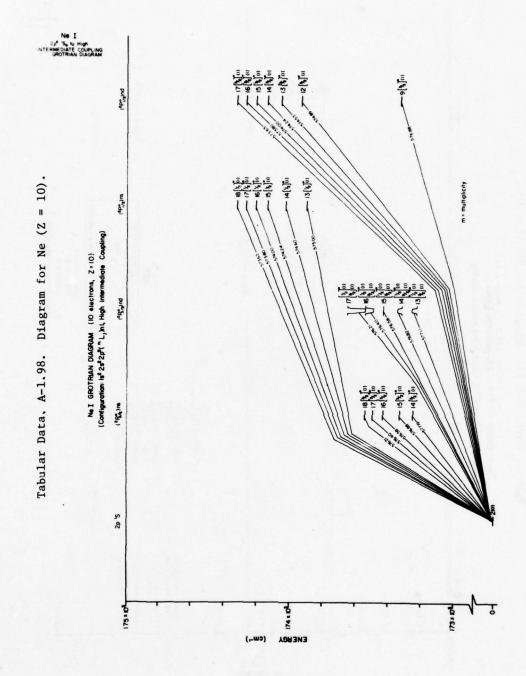
COTES: n!=2p*(2p**) n'!=2p*(2p**) n'f' [3] (3,4) Tabular Data. A-1.95. Diagram for Ne (Z = 10). Ne I GROTRIAN DIAGRAM (10 electrons,Z=10) (Configuration: 1s² 2s² 2p° (2P)nl,3p to Higher Terms) 72 (2.3) 74 (2.3) 75 (4.3) 75 (6.3) (10)[7], s,u ns 12 (2.1) TOx STI 65xIO



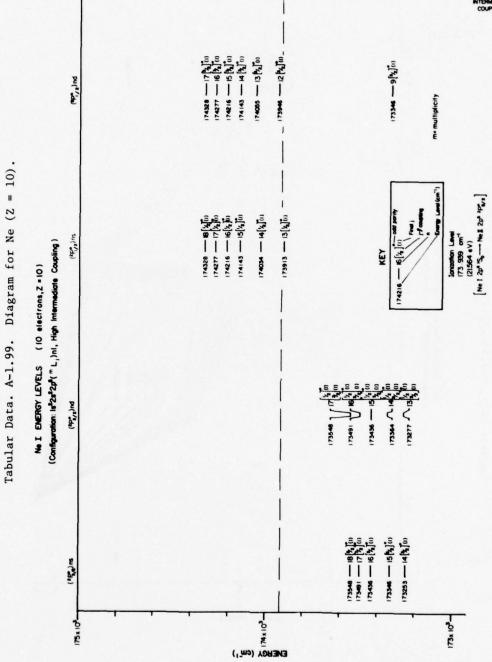


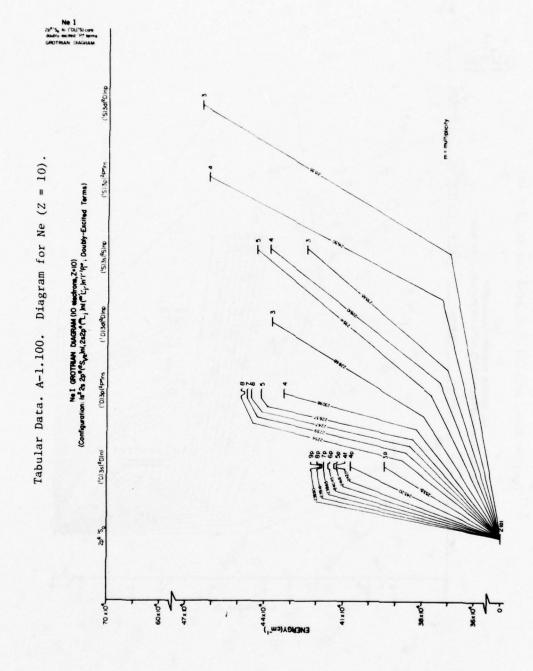
Tabular Data. A-1.97. Diagram for Ne (Z = 10).

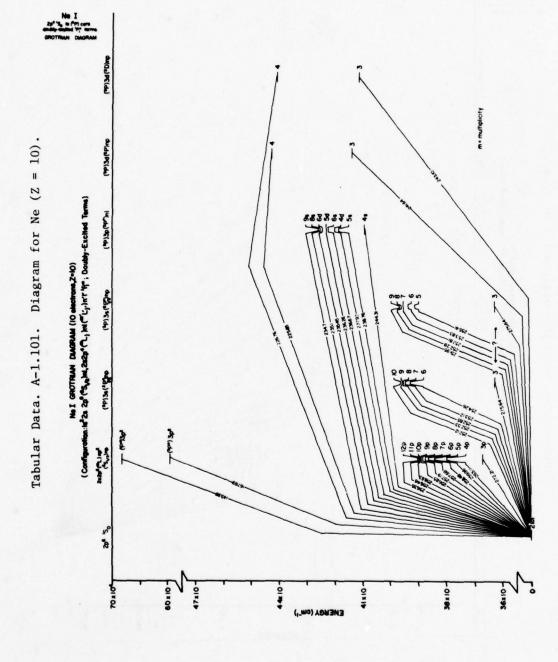




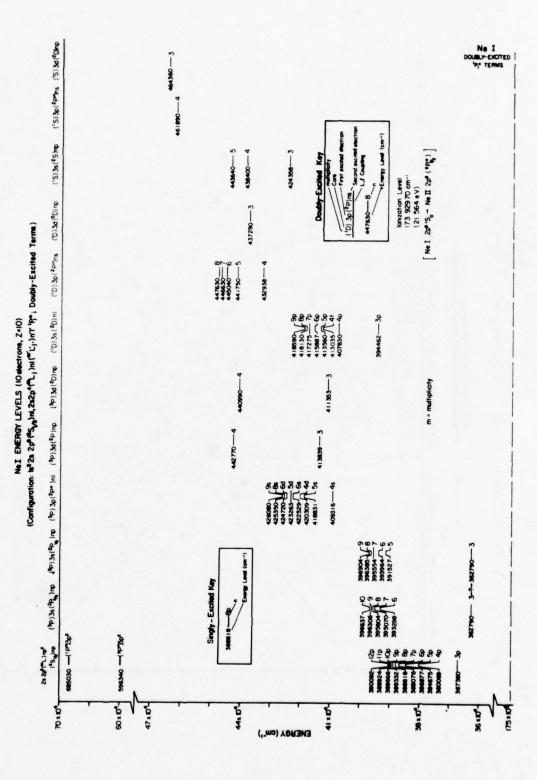
HIGH INTERNEDIATE COUPLING

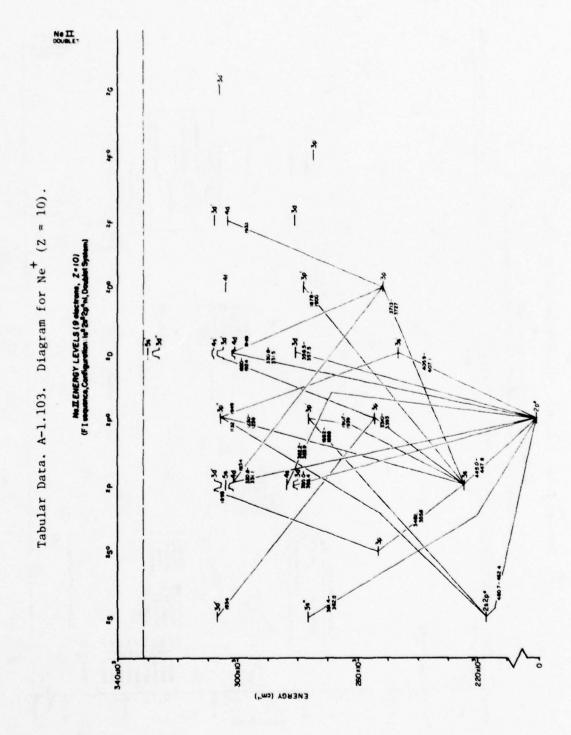




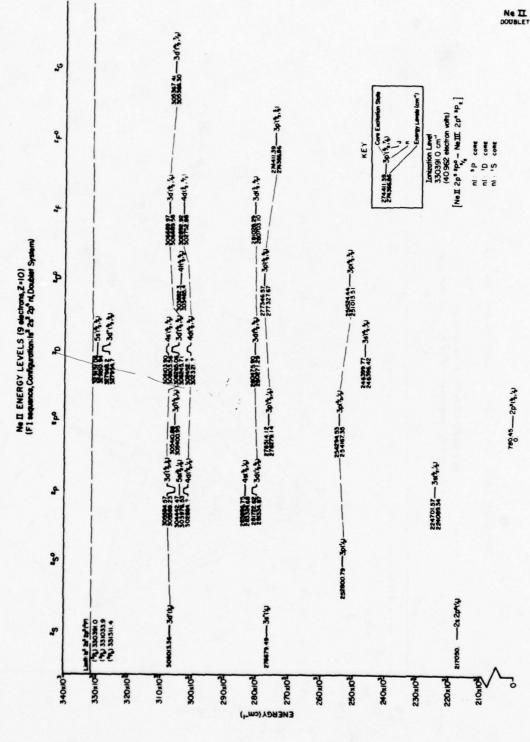


Tabular Data. A-1.102. Diagram for Ne (Z = 10).

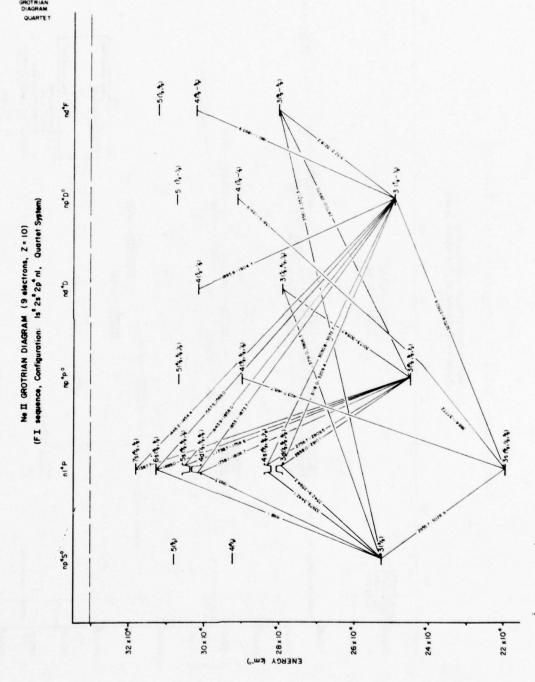




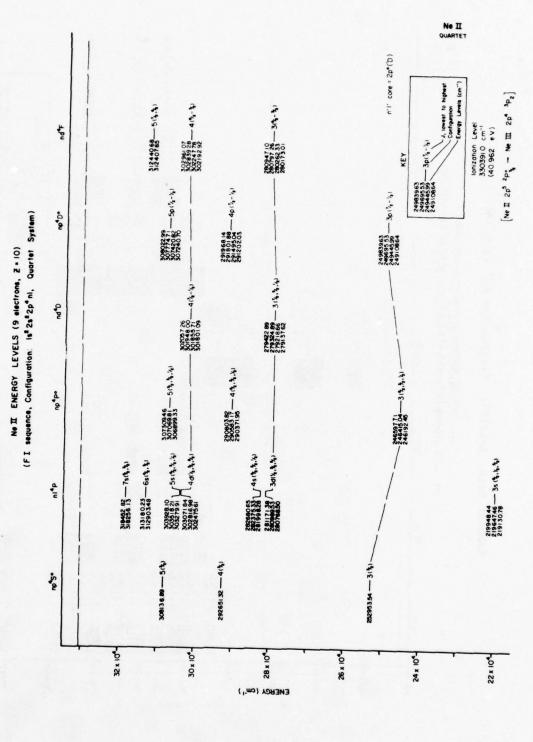
Tabular Data. A-1.104. Diagram for Ne⁺ (Z = 10).



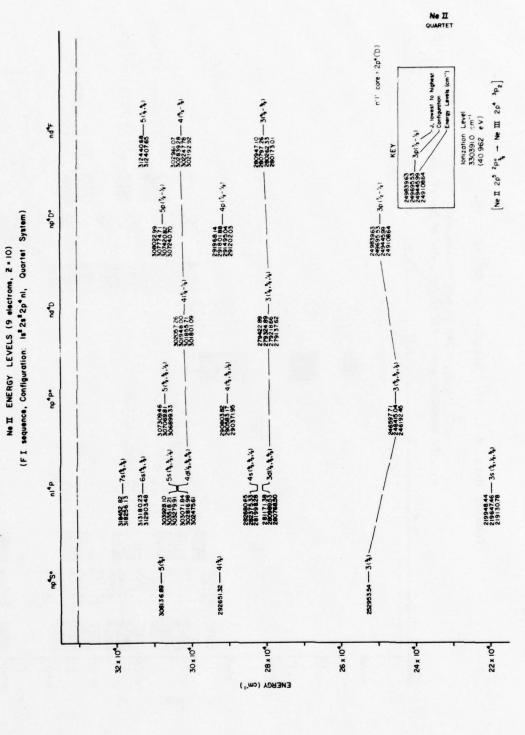
Tabular Data. A-1.105. Diagram for Ne (Z = 10).



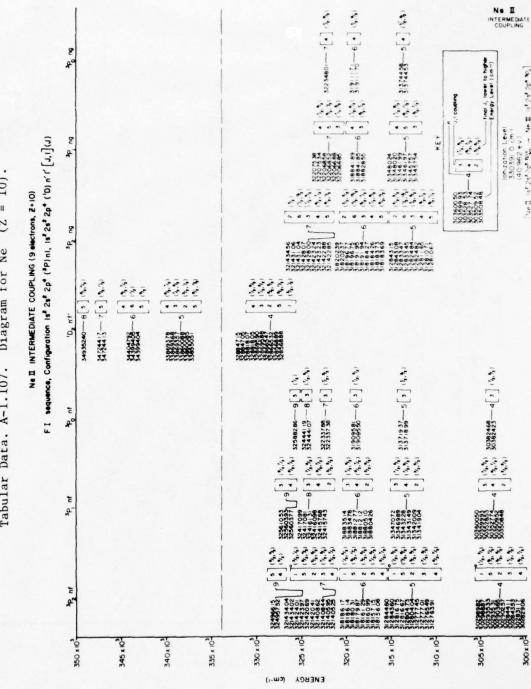
Tabular Data. A-1.106. Diagram for Ne (Z = 10).



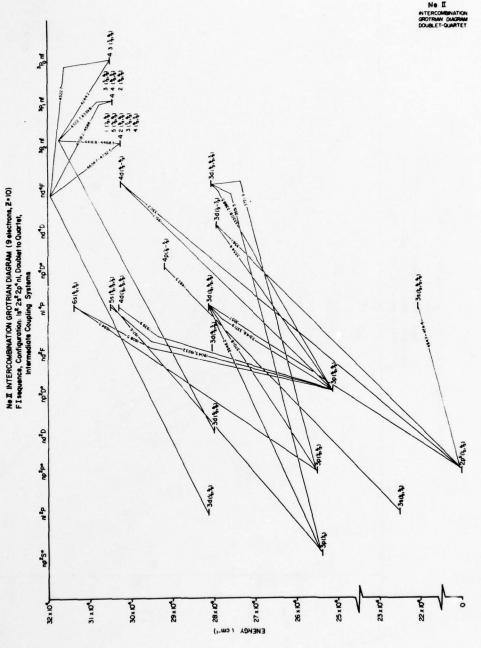
Tabular Data. A-1.106. Diagram for Ne $^+$ (Z = 10).



Tabular Data. A-1.107. Diagram for Ne⁺ (Z = 10).



Tabular Data. A-1.108. Diagram for Ne $^+$ (Z = 10).



Tabular Data. A-1.109. Diagram for Ne $^+$ (Z = 10). n core 20 (P) Ne I GROTRIAN DAGRAM (9electron, 2-10)
(F I sequence, Configuration is 2st 2pt in Courter to Doublets 8 intermediate Coupling , intercombination)

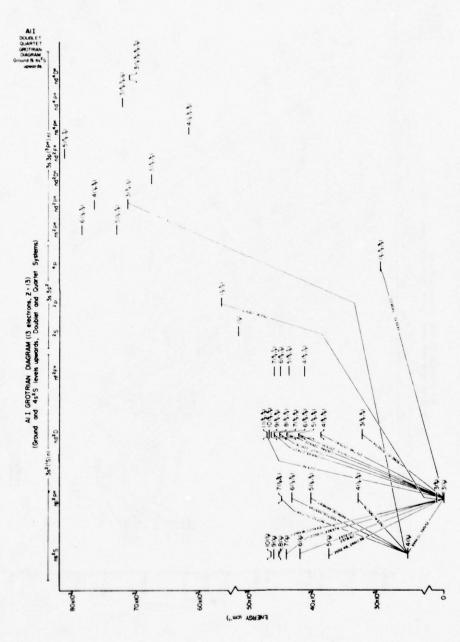
45

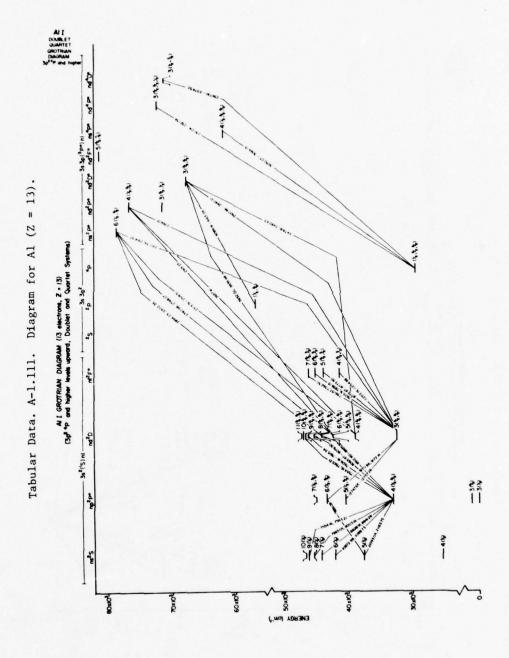
45

75

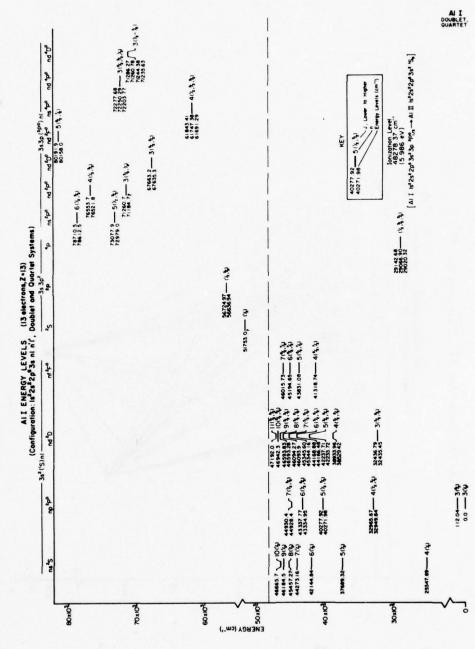
86 - 3p(1, 1) The second 4 Dane 305.0 2010 -0198 20.03 ENERGY (cm-1) 215.02 2010 28.0 20.02

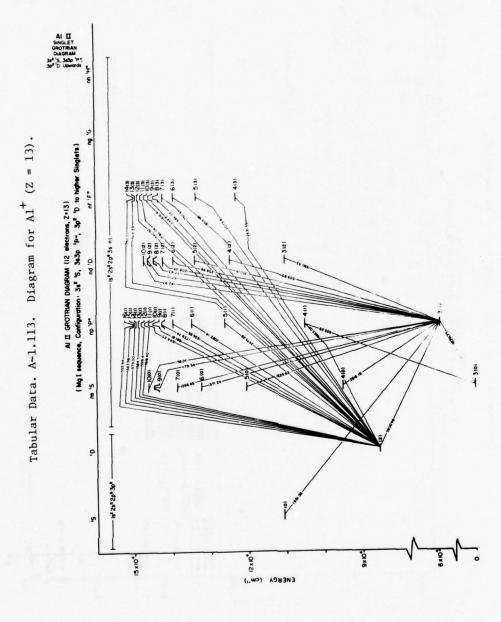
Tabular Data. A-1.110. Diagram for Al (Z = 13).



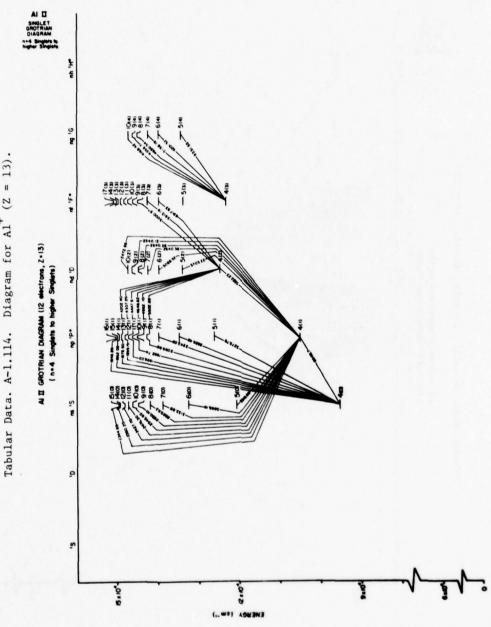


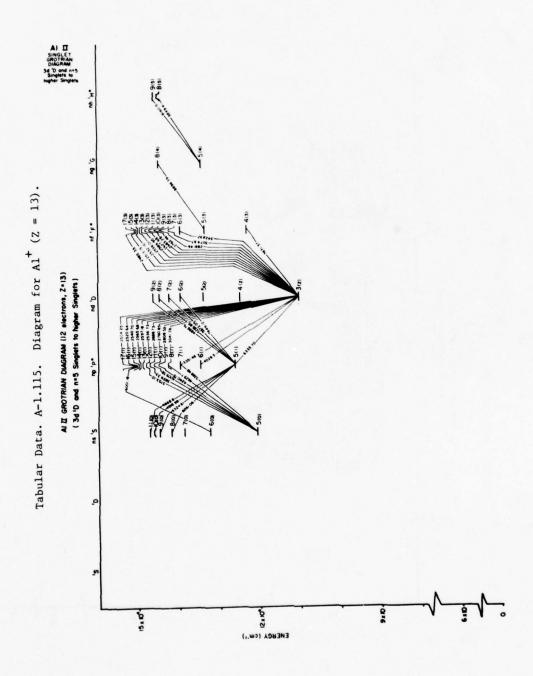
Tabular Data. A-1.112. Diagram for Al (Z = 13).



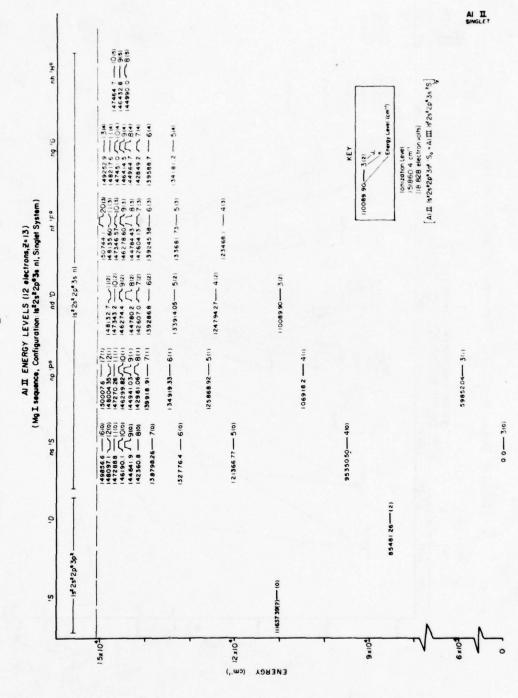


Tabular Data. A-1.114. Diagram for $A1^+$ (Z = 13).

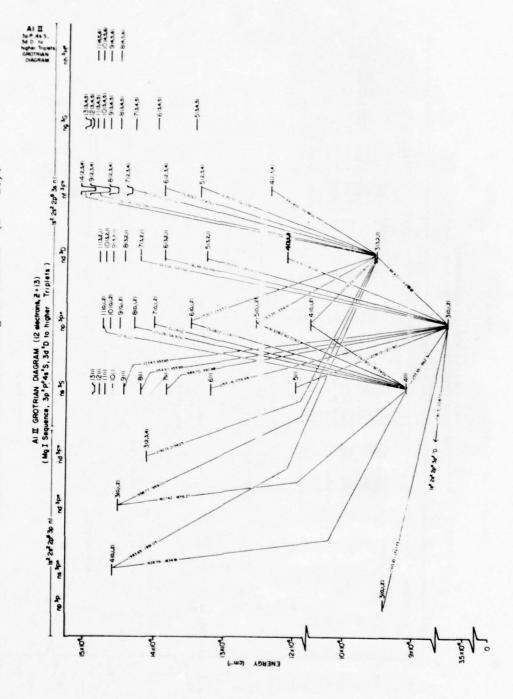




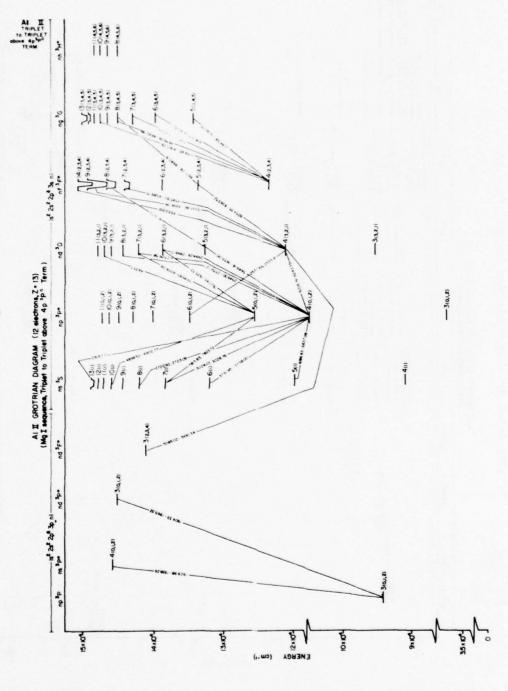
Tabular Data. A-1.116. Diagram for $A1^+$ (Z = 13).



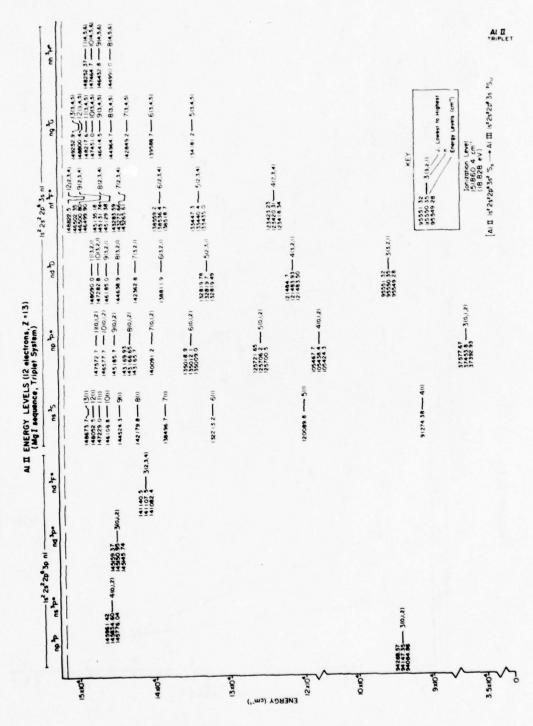
Tabular Data. A-1.117. Diagram for Al^+ (Z = 13).



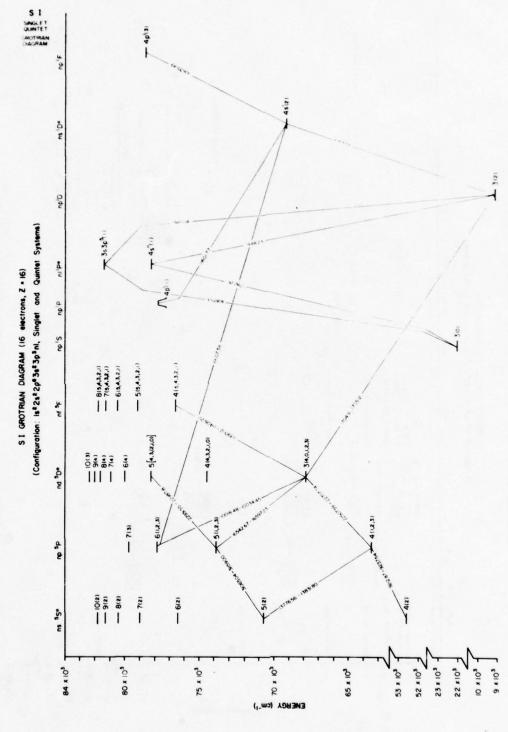
Tabular Data. A-1.118. Diagram for Al^+ (Z = 13).



Tabular Data. A-1.119. Diagram for $A1^+$ (Z = 13).



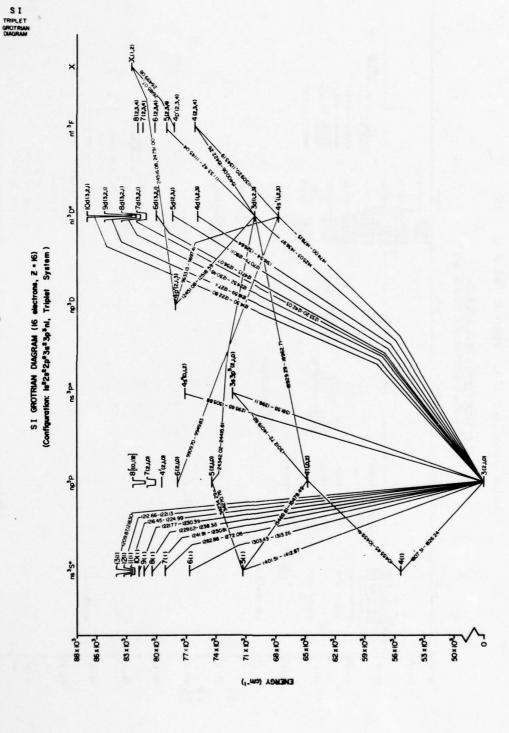
Tabular Data. A-1.120. Diagram for S(Z = 16).



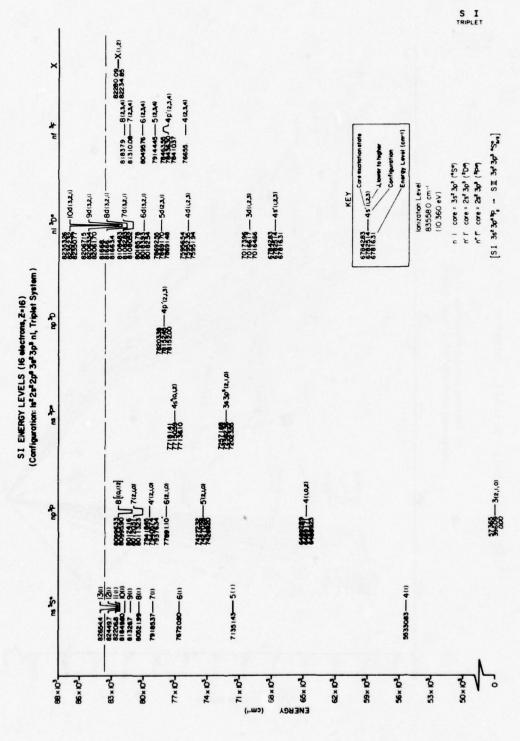
Tabular Data. A-1.121. Diagram for S (Z = 16).

S I SINGLETS QUINTETS 78638 2 - 4p(3 [51 35 36 36 - 51 35 36 35 [5] 69237.83 - 45(2) 00,50 ionzation Level 83 558 c cm⁻¹ (0.350 eV) ni circe - 3s² 3p¹(59) ni circe - 3s² 3p¹(59) ni circe - 3s² 3p¹(59) 923658 -- 3(2) 00 S Z ENERGY LEVELS (16 electrons, Z*16) (Configuration is 2s² 2p² 3s² 3p³ nl, Singlet and Quintet Systems) 8:4374 - 353090 7828642 — 45°(i) 77853956 \(\textstyle Ap\(\text{(i)} \) 0d, N d, o S, du 8130923 — 8154532.01 8130923 — 715,4532.01 8049473 — 615,4532.01 76653 - 4(5,4.3.2.1) 7914318 - 5(5,4,3,2,1) 79) 77857030 — 5(4,32,0) 77857030 — 5(4,32,10) 7497690 7497631 7591516 — 50.2.31 7497335 7391150 8205394 — 9(4) 8162890 — 9(4) 8099548 — 7(4) 7999236 - 6(4) on spo 63475 26 63457 33 — 4 (, 2, 3) 63446 36 de du 8181940 — 10(2) 8128176 — 9(2) 8044930 — 8(2) - 5(2 7905824 - 7(2) 7646426 -- 6(2) 5262365 - 4/Z 05° SU 6 1103 J 84 x 103 80 x 103 76 x 103 ENERGY (cm-1) 64 x 103 53 x 103 -10 x 103 23 x 103 22 x103 72 x 103 52 x 103

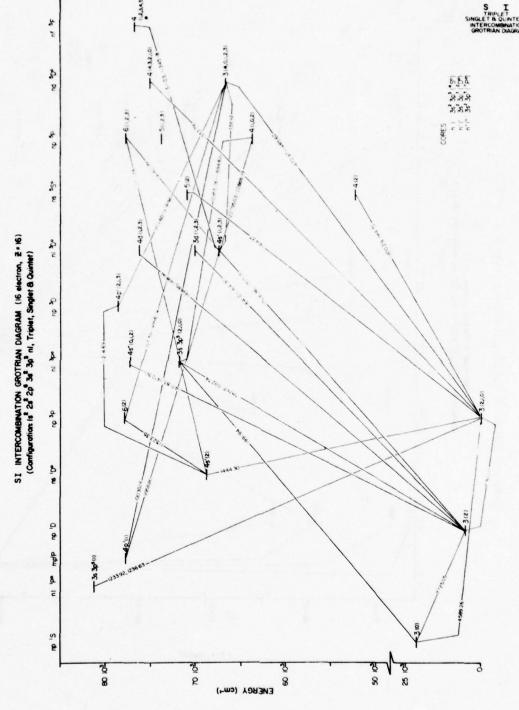
Tabular Data. A-1.122. Diagram for S(Z = 16).



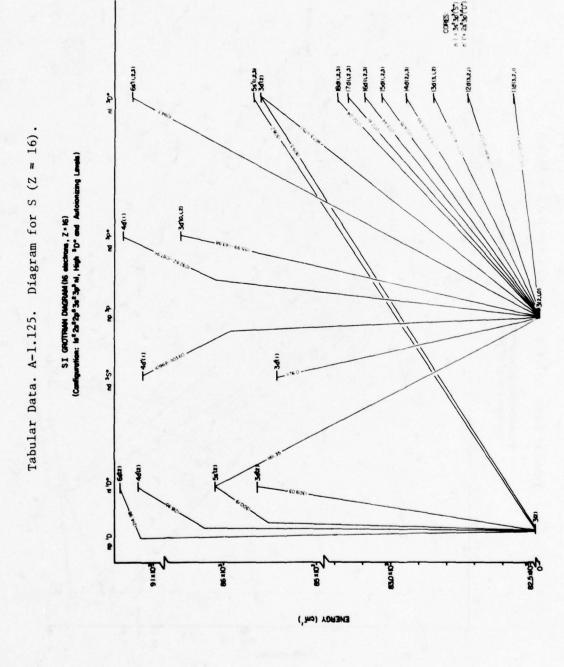
Tabular Data. A-1.123. Diagram for S (Z = 16).



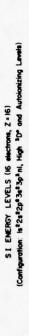
Tabular Data. A-1.124. Diagram for S(Z = 16).

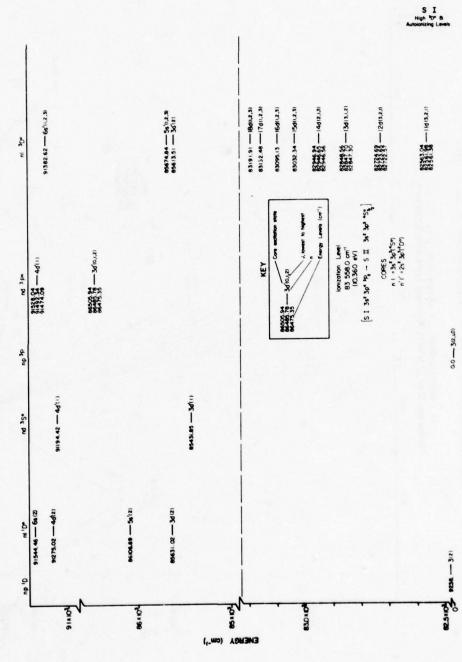


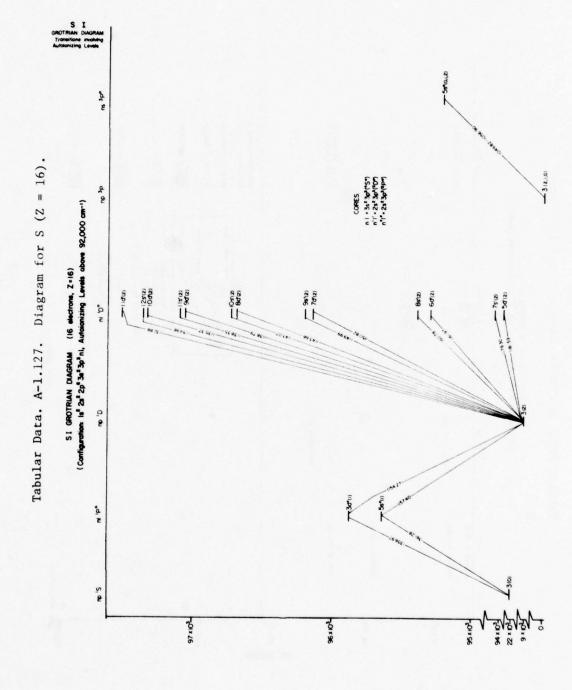




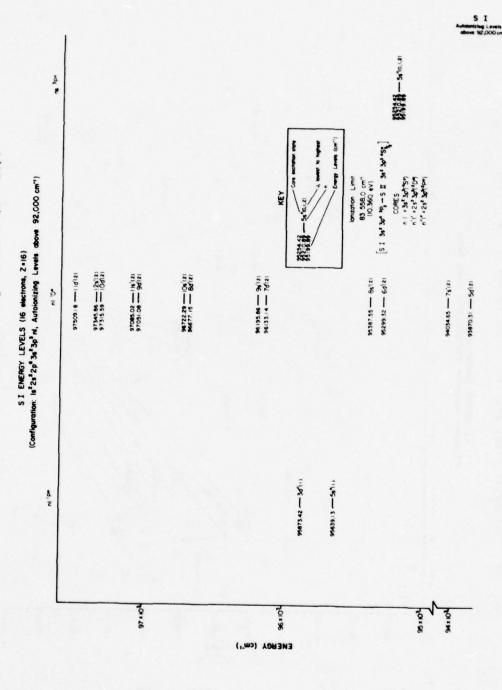
Tabular Data. A-1.126. Diagram for S(Z = 16).

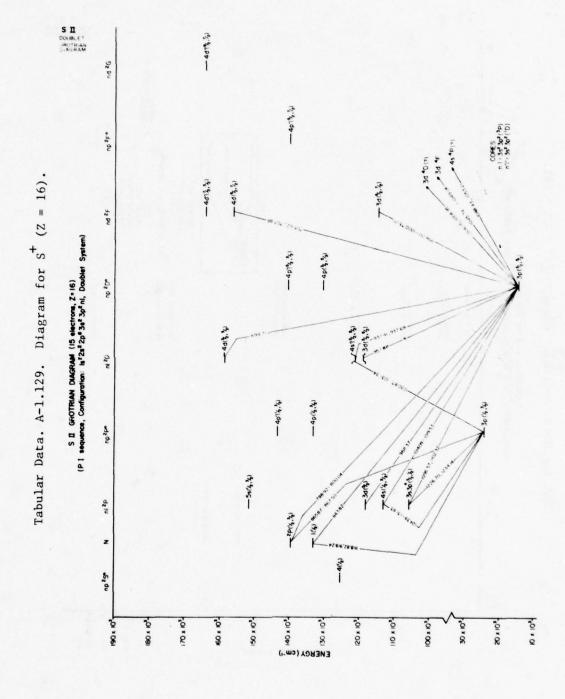






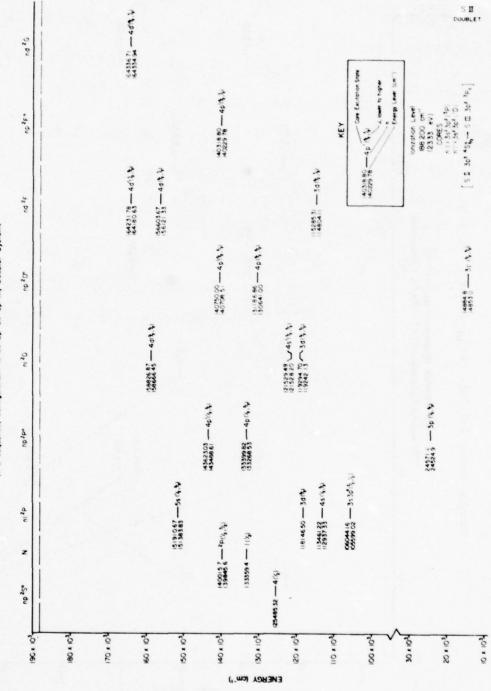
Tabular Data. A-1.128. Diagram for S(Z = 16).

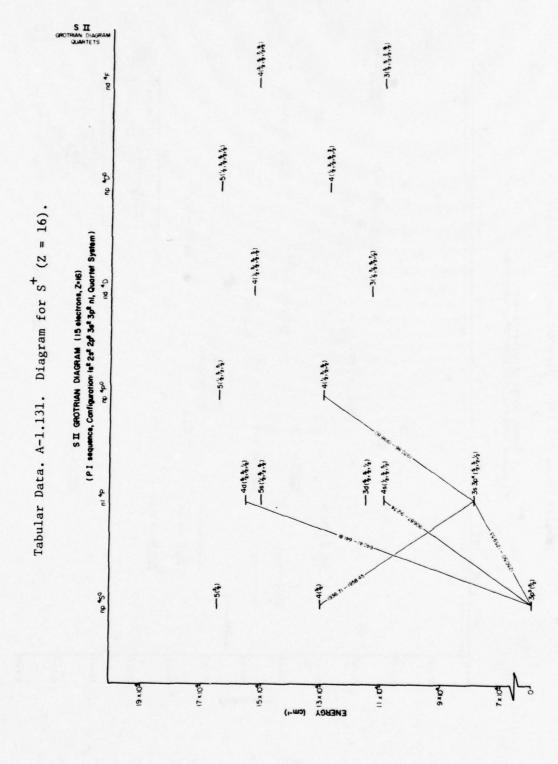




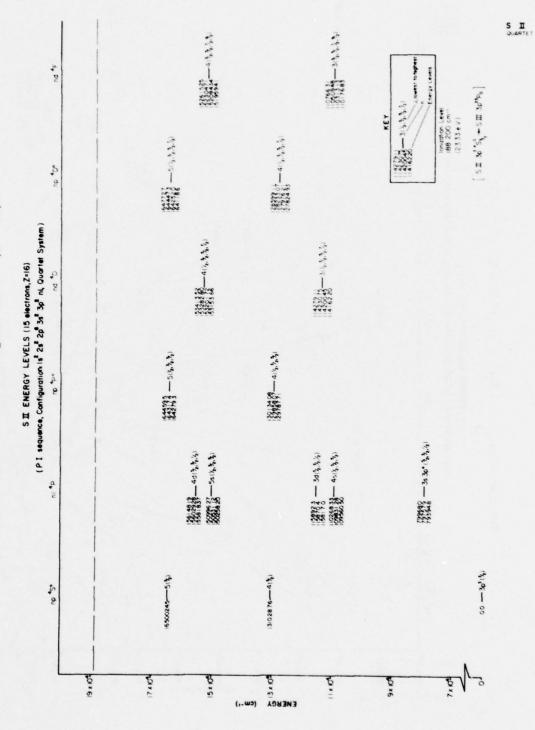
Tabular Data. A-1.130. Diagram for S^+ (Z = 16).

S II ENERGY LEVELS (15 electrons, Z = 16)
(P I sequence, Configuration: 18²2s²2p⁶3s²3p²nl, Doublet System)

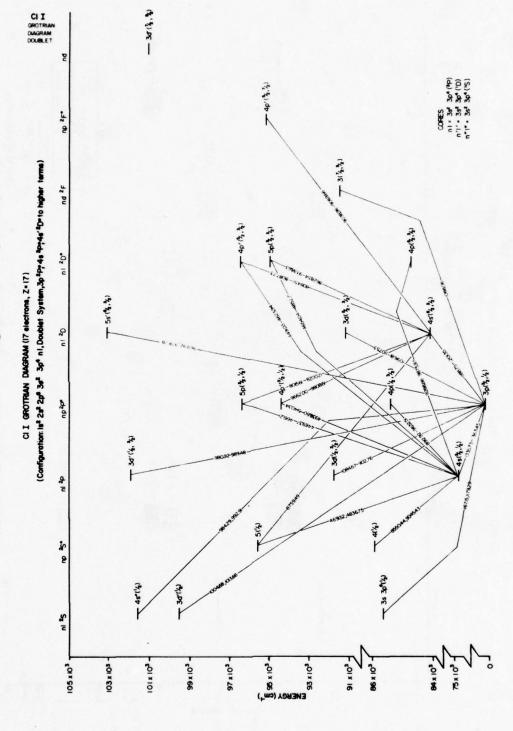




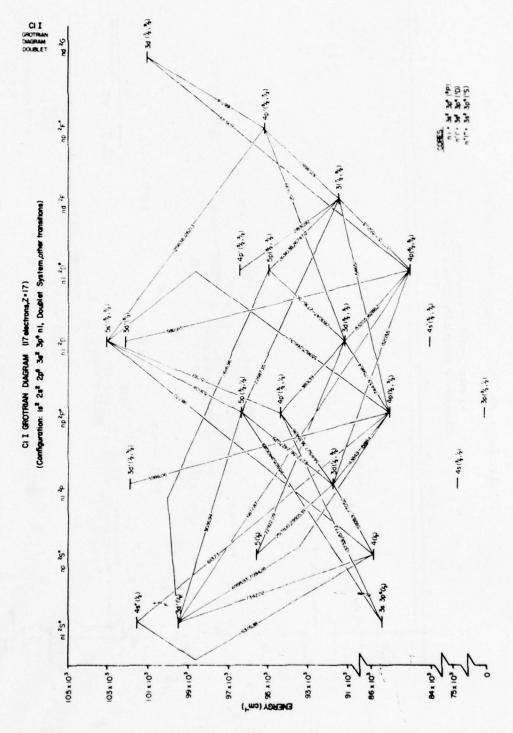
Tabular Data. A-1.132. Diagram for S^+ (Z = 16).



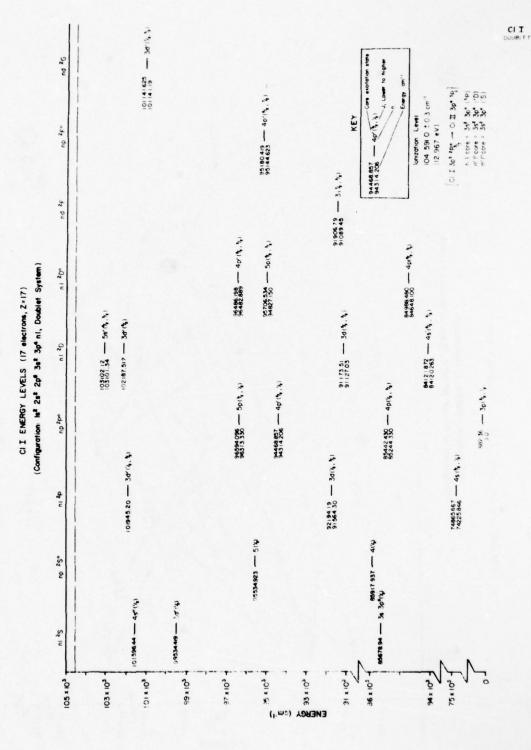
Tabular Data. A-1.133. Diagram for C1 (Z = 17).

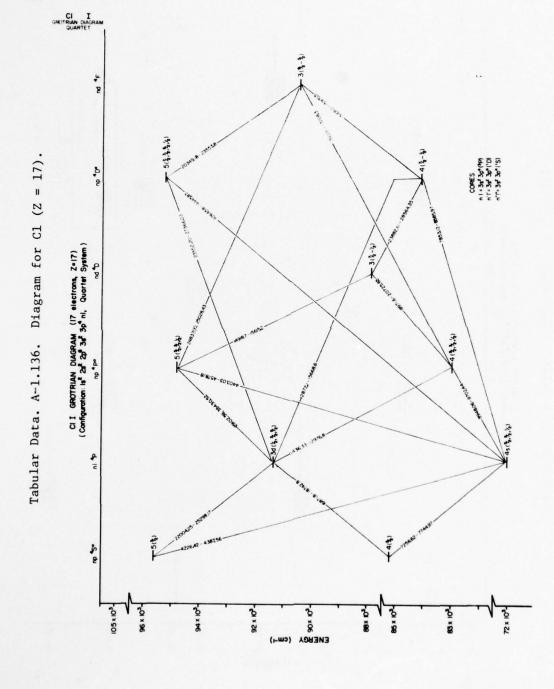


Tabular Data. A-1.134. Diagram for Cl (Z = 17).

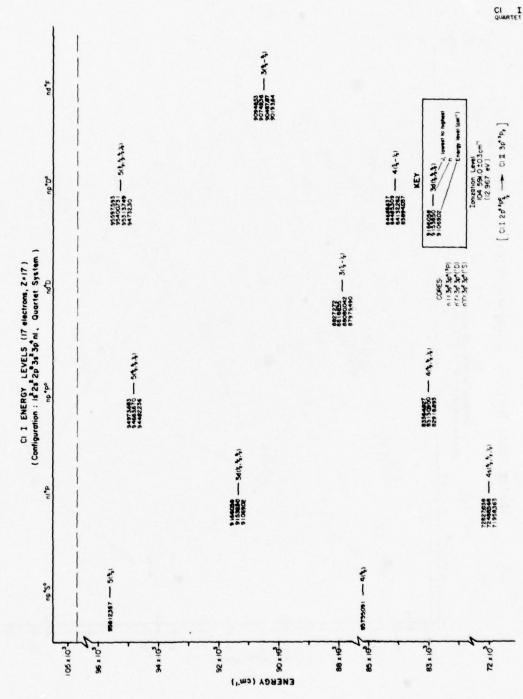


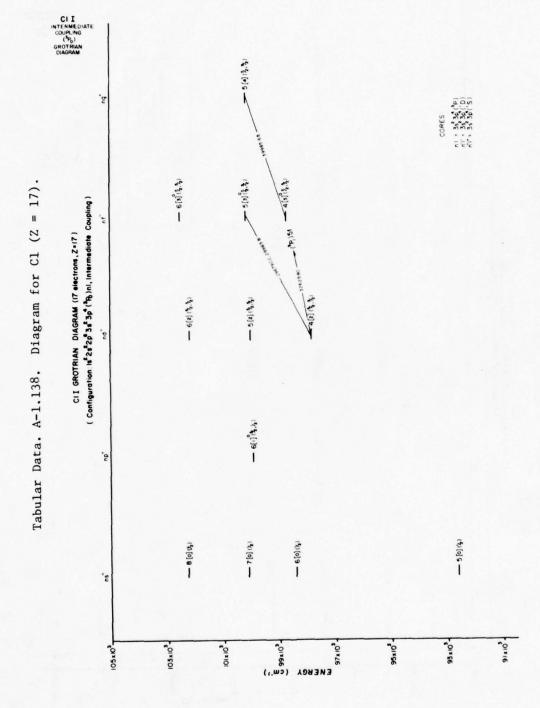
Tabular Data. A-1.135. Diagram for C1 (Z = 17).



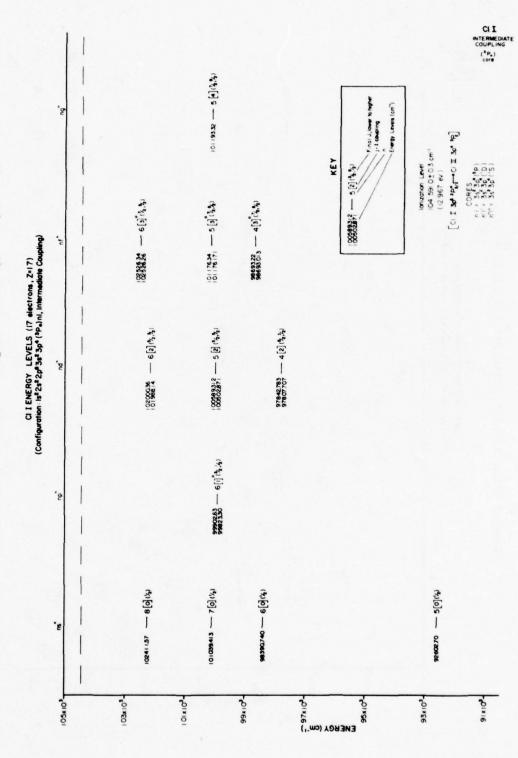


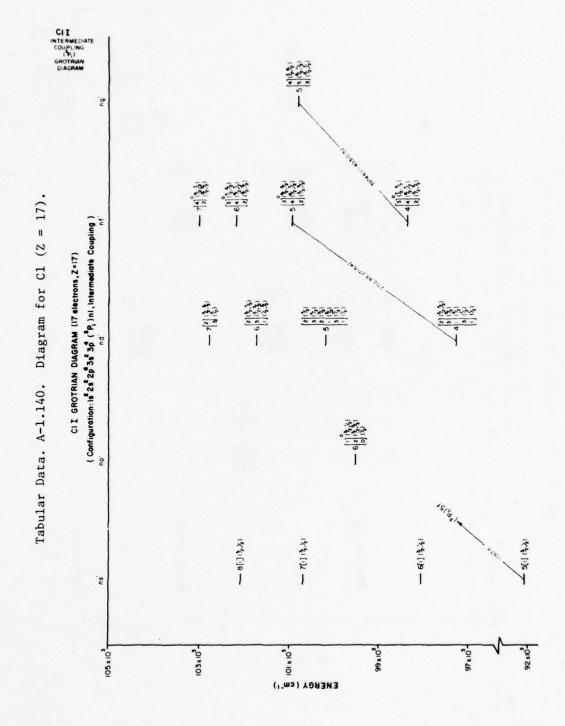
Tabular Data. A-1.137. Diagram for C1 (Z = 17).



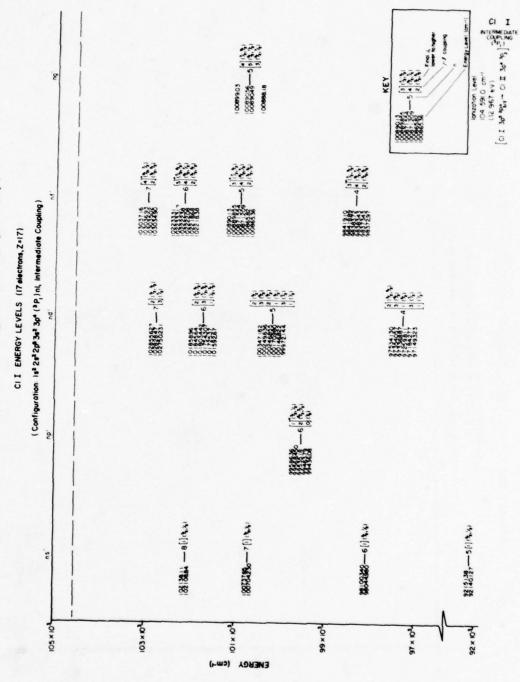


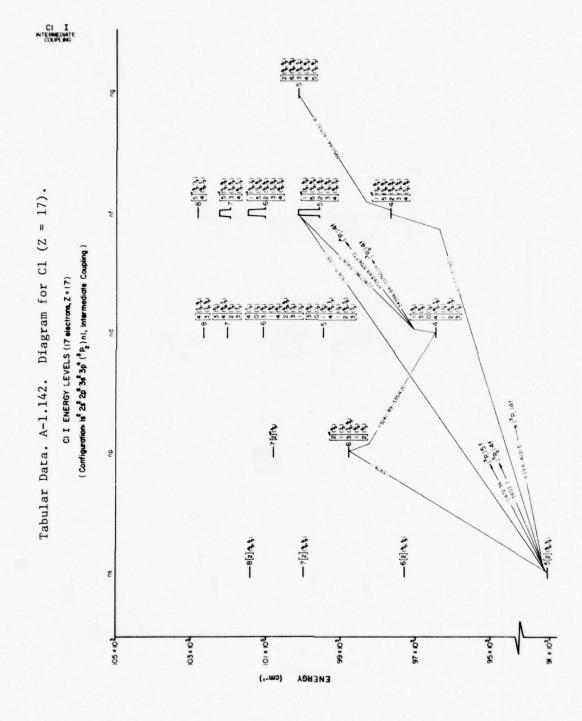
Tabular Data. A-1.139. Diagram for (Z = 17).



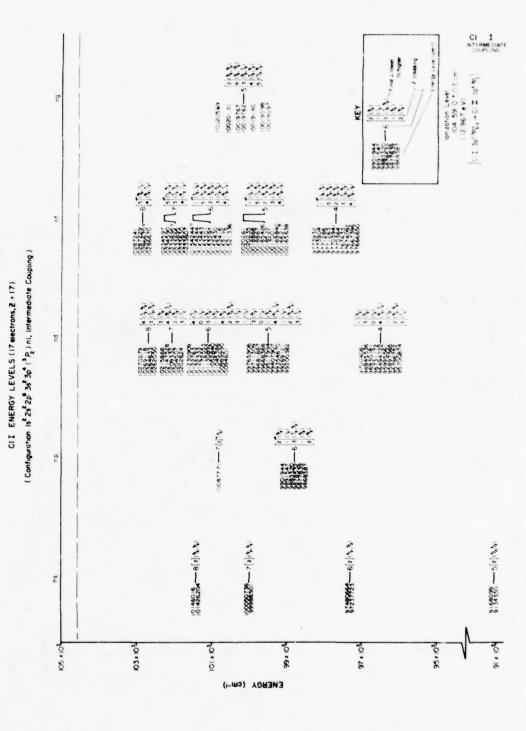


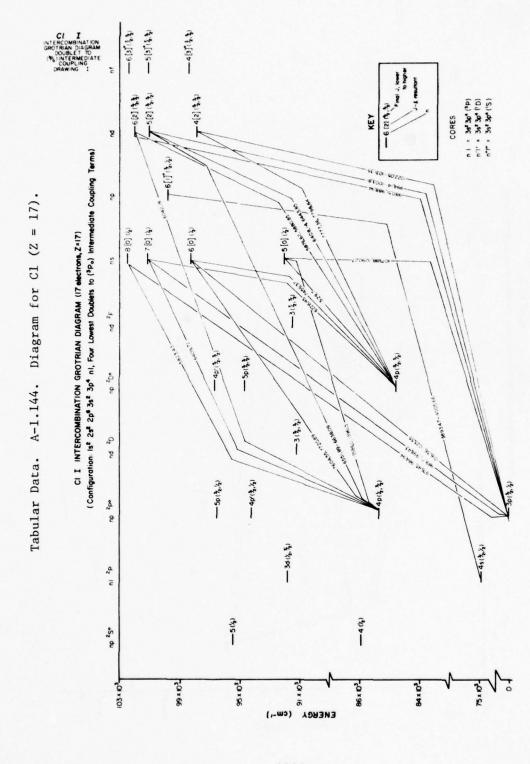
Tabular Data. A-1,141. Diagram for (Z = 17).





Tabular Data. A-1.143. Diagram for C1 (Z = 17).





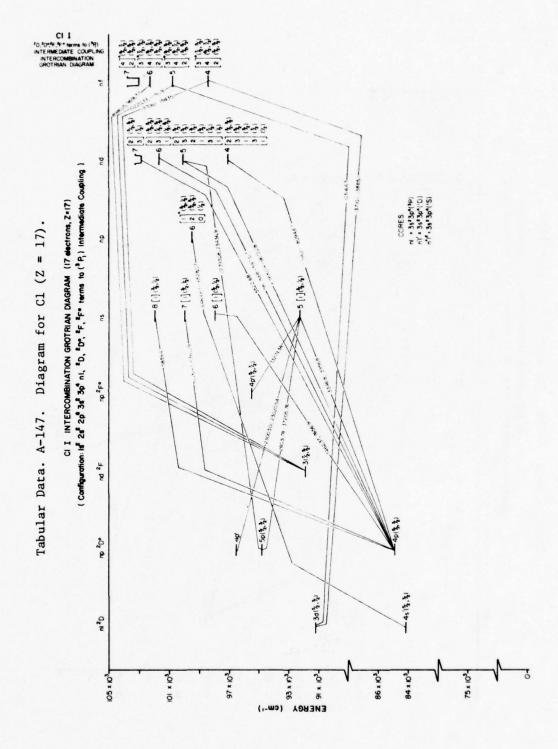
-6[3](2,2) -5[3] (3,\$) 7-4[3](3,3) -5[2] (\$.\$) -4[2] (\$.\$) -6[2] (\$,\$) P CORES IN LS COUPLING II | 3830 (P) II | 3830 (S) đ CI I INTERCOMBINATION GROTRIAN DIAGRAM (17 electrons, Z=17) (Configuration: \mathbf{ls}^2 \mathbf{Zs}^2 \mathbf{Zp}^6 $\mathbf{3s}^2$ $\mathbf{3p}^6$ n., Transitions Between 4p 2 S° or Higher Doublets and Intermediate Coupling Terms) Tabular Data. A-1.145. Diagram for C1 (Z = 17). (4) [0] 8— 7[0] (%) (4) [0]9 -5[0](%) nd 2F 40 (3.2) - 4p(\$,\$) np 200 £3(2,2) og pu -20(3.4) £40(2,4) -4p(1,1) -30(\$,1/2) 20 -661127, 7073.76 -34 (\$, \$) 45 (\$, 1/2) 1 2p (2)5 no So 103×101 -01×66 95 x 103-ر چ چ ENERGY (cm-1) 84×103-86x103 75×10-

1044

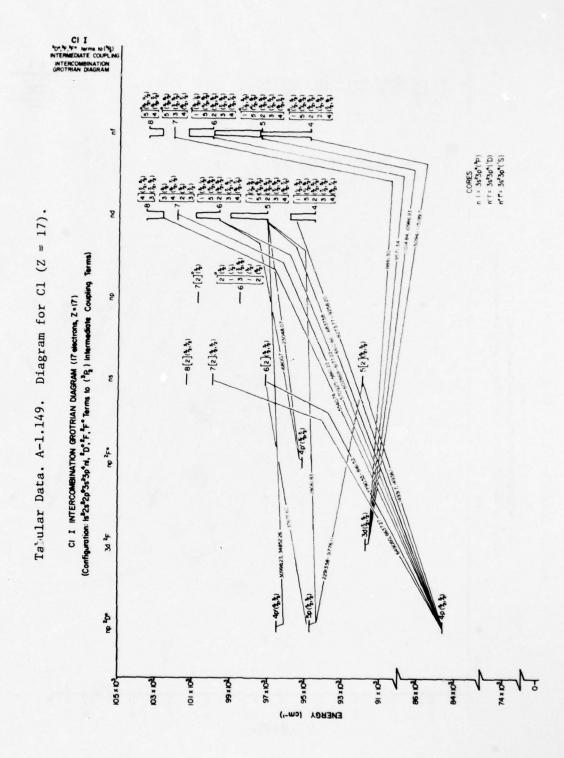
CORES nl = 3s²3p⁶(²P) nl' = 3s²3p⁶('S) nl' = 3s²3p⁶('S) CI INTERCOMBINATION GROTRIAN DIAGRAM (17 electrons, Z=17) (Configuration: is 2s2 2p2 3s2 3p2 n1, 85°, 2p, 5pc terms to (2 p) Intermediate Coupling) 5 Tabular Data. A-146. Diagram for Cl (Z = 17). d c (34) [1] 9-(4.4)[1] SC 40(4,4) 45. (4.4.) of odz du - 30 (x, x) 5 9 .S₂ du ENERGY 105 x 10² 91 x 103-86 x 103-0 × 10 ₹0 × 26 84 × 104 75 x 104 (cw-1)

CI I

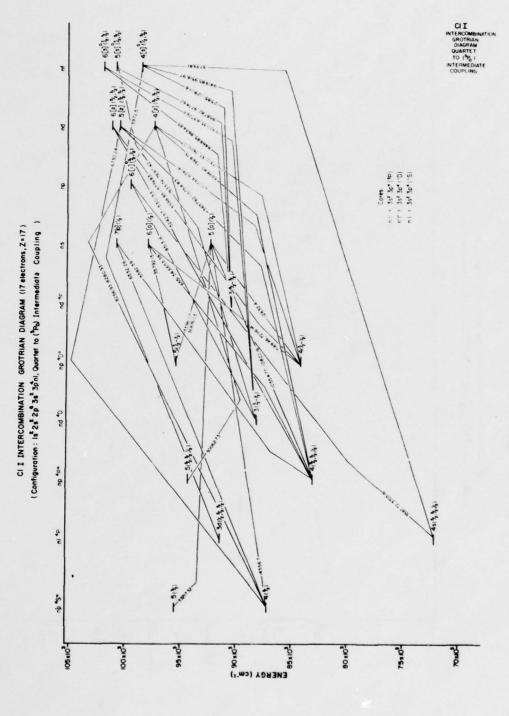
S, *P, *P* terms to (*P,)
INTERMEDIATE COUPLING
INTERCOMBINATION
GROTRIAN DIAGRAM



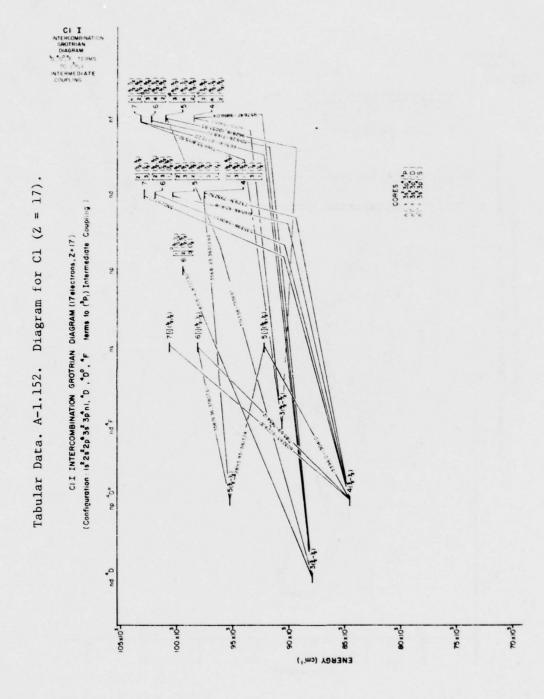
CI I INTERCOMPINATION GROTIAN DIAGRAM *2c *p* to *0 terms 2 Tabular Data. A-1.148. Diagram for C1 (Z = 17). CI I INTERCOMBINATION GROTRIAN DIAGRAM (17 electrons, Z=17) (Configuration: 1s² 2s² 2p³ 3s² 3p² ni, ²S; ² p;² Po²D terms to (³P₂) Intermediate Coupling) đ - 8[2](\$,\$) 7-6[2]18.2) 5[2](3,3) 7[2](3,3) S - 45 (2,3) 40(1,4) 2 du -45(\$,4) (4,4)05 nl 2p 1 5(%) °5, du 105 x 103 96x 103 74 x 103 101 x 103 Sox 103 91 x 103 84×103 103 x 103 97×103 95 x 10 93 x 103 ENERGY(cm⁻¹)

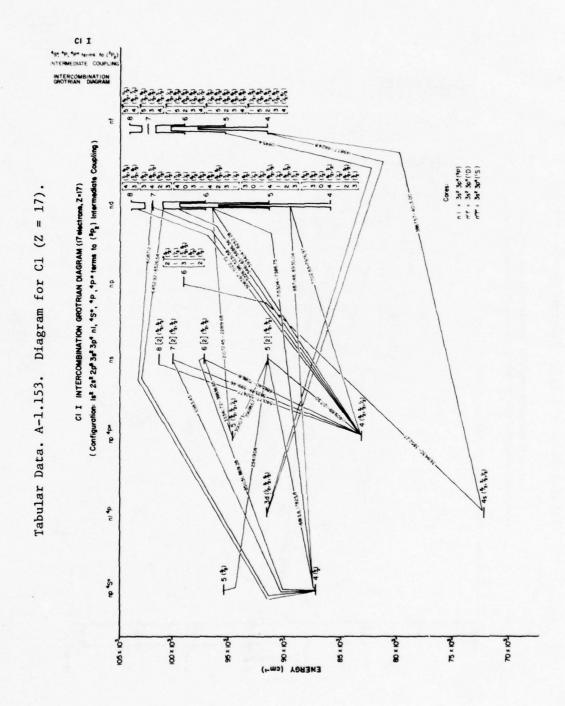


Tabular Data. A-1.150. Diagram for Cl (Z = 17).



Intermediate Coupling Cores n I = (%) n P = (%) Tabular Data. A-1.151. Diagram for C1 (Z = 17). CI I INTERCOMBINATION GROTRIAN DIAGRAM (17 electrons, Z=17) (Configuration: 13 23 22 33 35 11, 45° 40, 49° terms to (Pt.) Intermediate Coupling.) 71:32 34 (F) 30(2,2,2) S, du 105×10 OXOO! 95×103 ENEBGA (cm.,) 70x103 90x10 -01x 08 75x10-





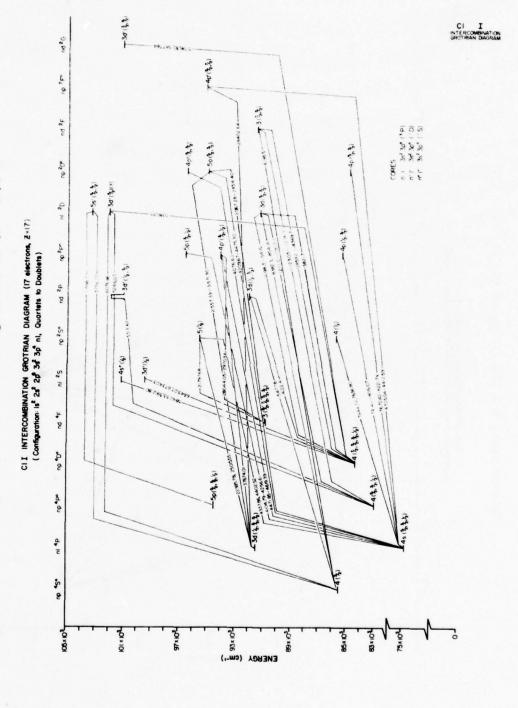
CI I
INTERCOMBINATION
GROTRIAN
DIAGRAM

(*D,*D*,*F terms to
(*P₂) intermediate (Configuration: Is² 2s² 2p² 3s² 3p² ni, *D, *D°, *F terms to (*Pg.) Intermediate Coupling terms) 696.32 596.4.70.53 7360.44.759.83 690.48.89.82 10250 50-0600 50-Tabular Data. A-1.154. Diagram for C1 (Z = 17). CI I INTERCOMBINATION GROTRIAN DIAGRAM (17 electrons, Z=17) 5 [2 (\$ \$) 2) --- 8 [2] (\$,\$) 7 [2] (\$,\$) - 6[2] (\$ \$) nd 4F CORES. n | = 35°30°(PP) n'| = 35°30°('D) n'| = 35°30°('S) ob du 5 105 x 10³ -00 x 00 95 x 103 75 × 10± 70 × 10 85 x 10³ 90 x 06 00 x 06 ENERGY

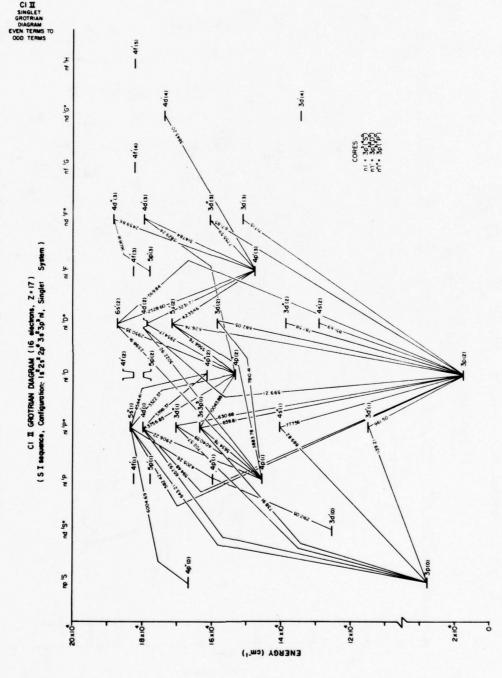
00,00 40 5(2.2.4) Diagram for C1 (Z = 17). od du J 30(4.3.3.) CI I INTERCOMBINATION GROTRIAN DIAGRAM (IT electrons, Z = 17) (Configuration: 1st 2st 2pt 3st 3pt nl, Doublet to Quartet) 1215 os du nd 2F Tabular Data. A-1.155. -34(4,4) -34(4,4) 050m o_lu np 2 P° ul Sp Se

CI I
DOUBLET to QUARTET
INTERCOMBINATION
GROTRIAN DIAGRAM 39.3.3.3 nd 4F CORES (1 = 35 30 (P) (1 = 35 30 (D) (1 = 35 30 (S) - 48(2,2,4) ENERGY (cm⁻¹) 88 x 103 72 x 10-96x10 92 x 103

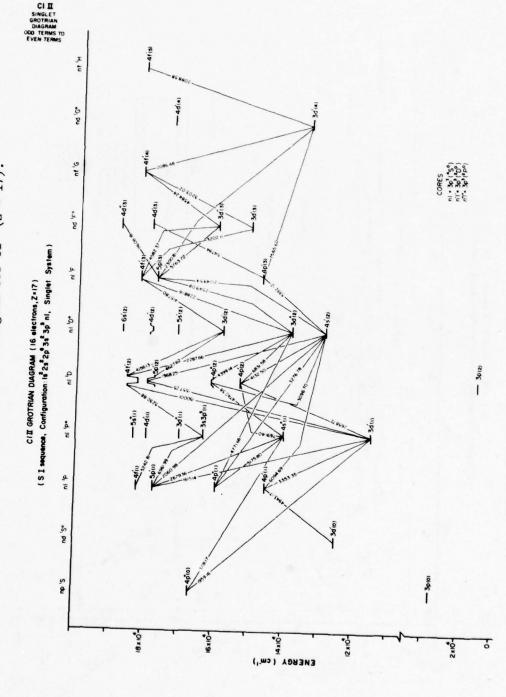
Tabular Data. A-1.156. Diagram for (Z = 17).



Tabular Data. A-1.157. Diagram for $C1^+$ (Z = 17).



Tabular Data. A-1.158. Diagram for $C1^+$ (Z = 17).

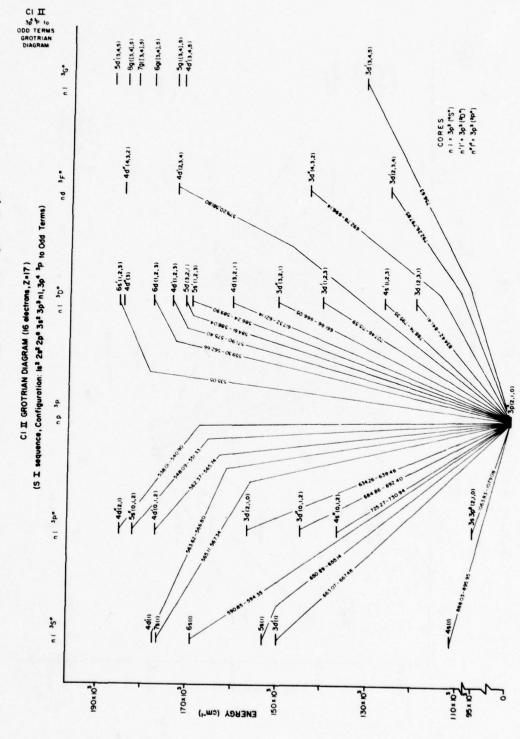


CI II

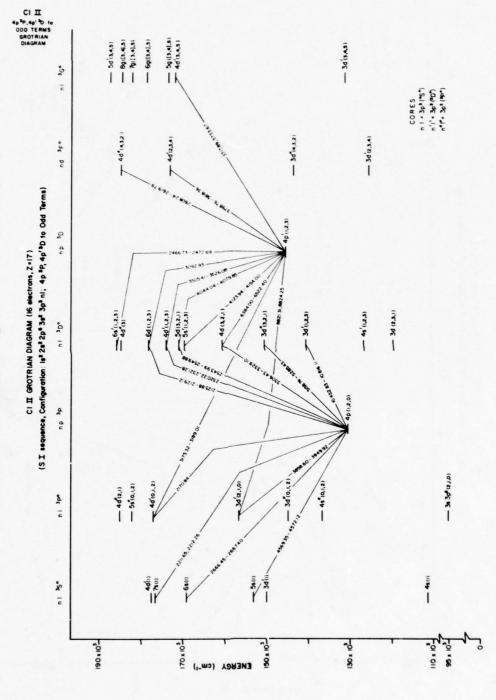
Tabular Data. A-1.159. Diagram for $C1^+$ (Z = 17).



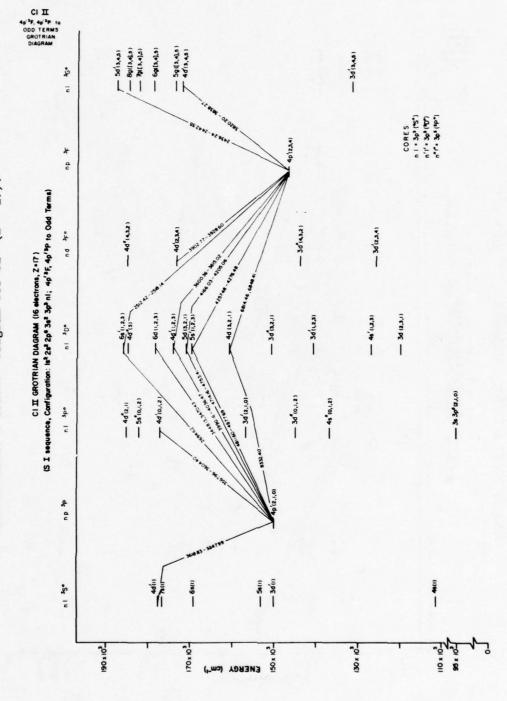
Tabular Data. A-1.160. Diagram for $C1^+$ (Z = 17).



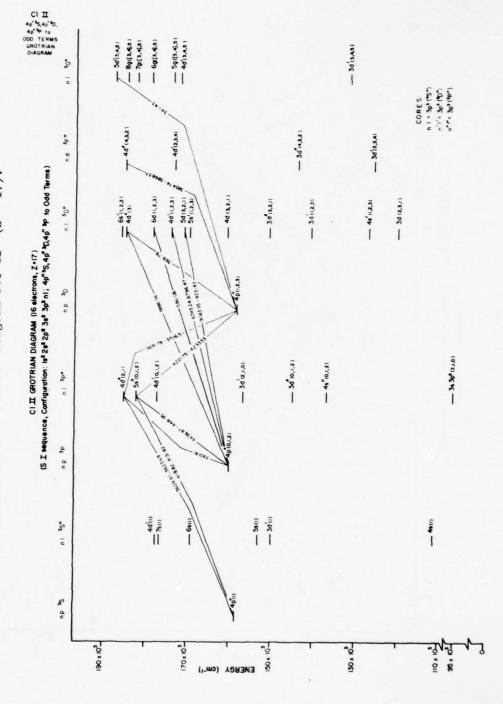
Tabular Data. A-1.161. Diagram for $C1^+$ (Z = 17).

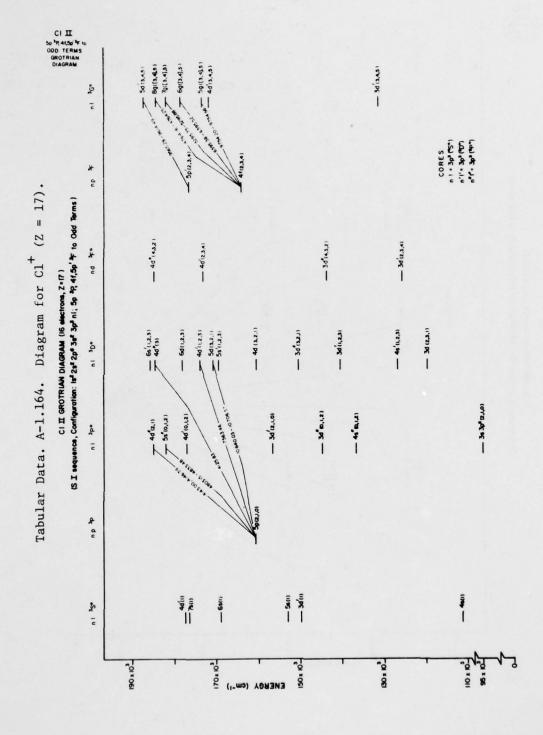


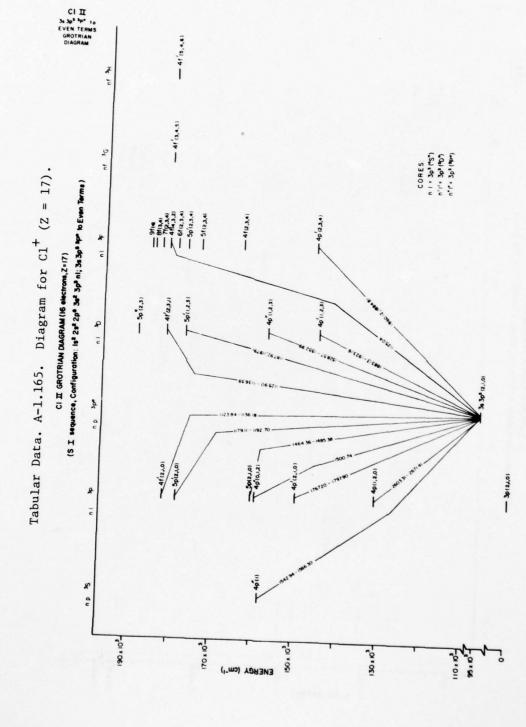
Tabular Data. A-1.162. Diagram for $C1^+$ (Z = 17).

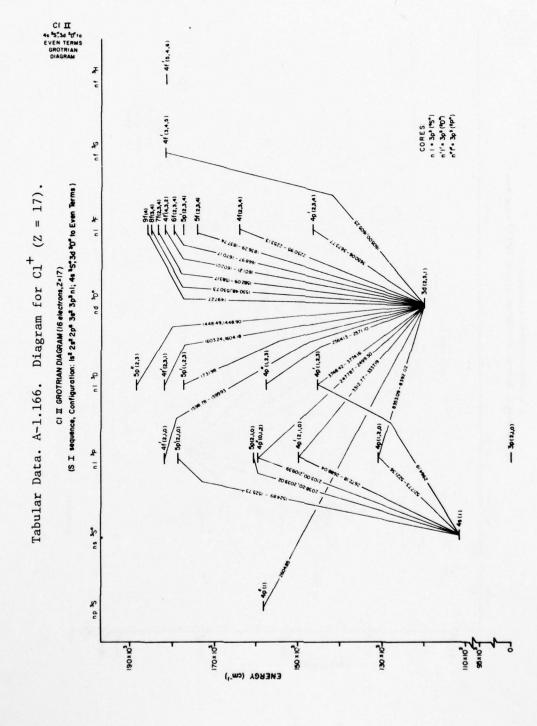


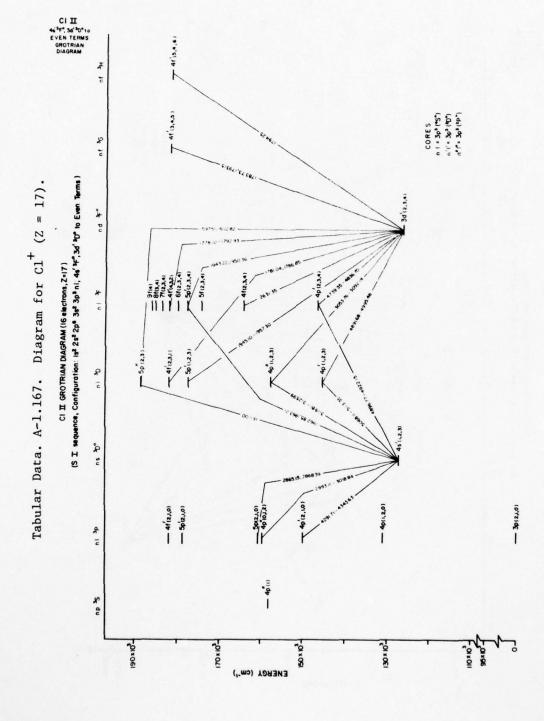
Tabular Data. A-1.163. Diagram for Cl^+ (Z = 17).

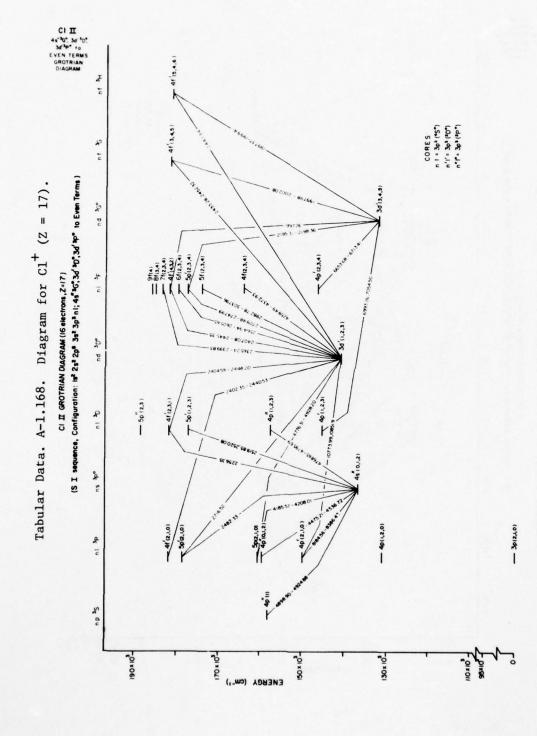


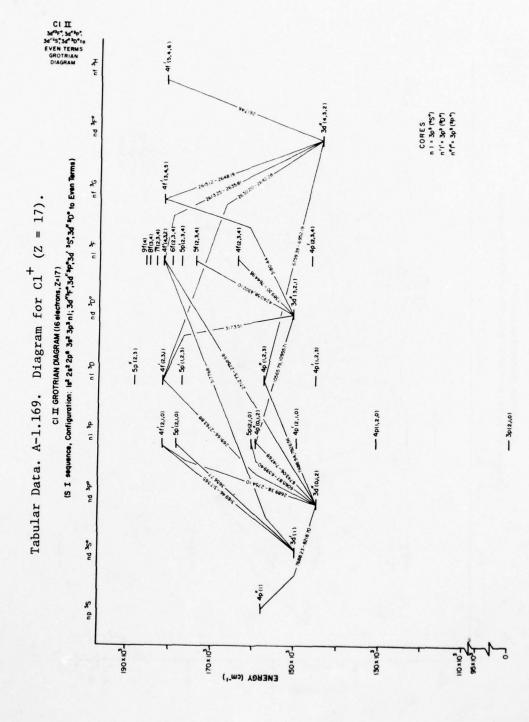


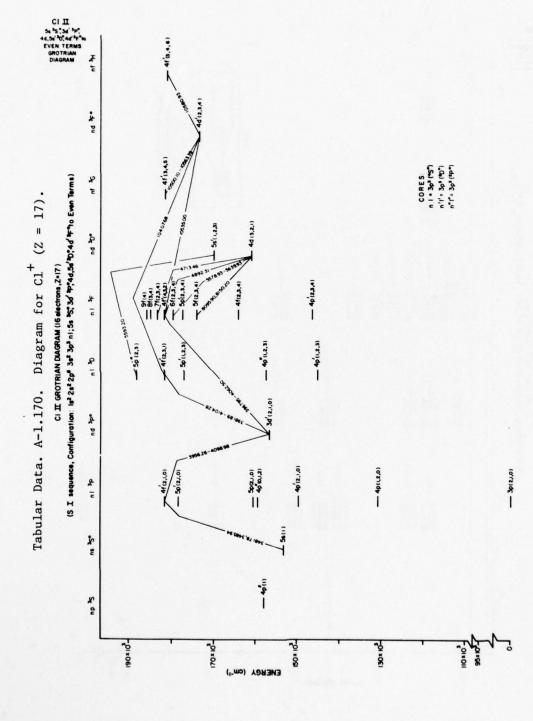


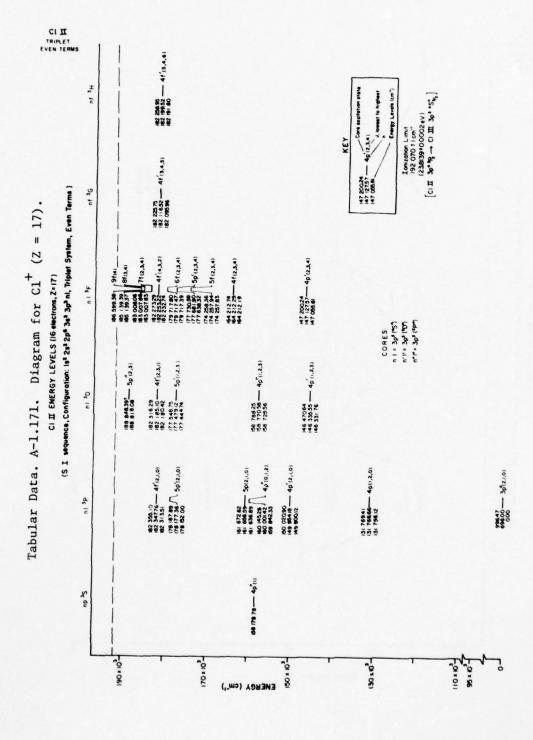




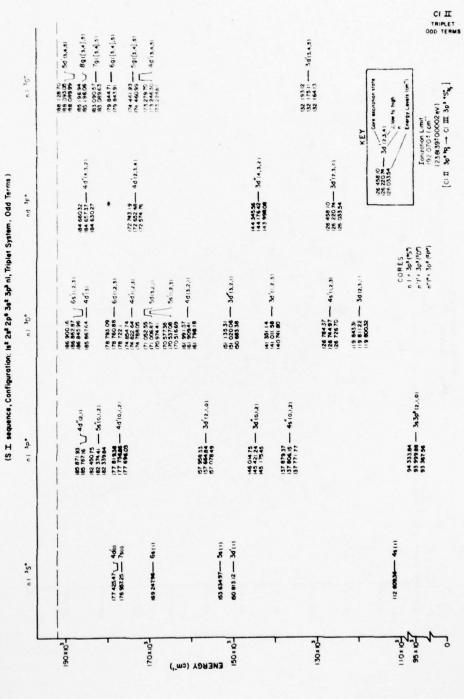


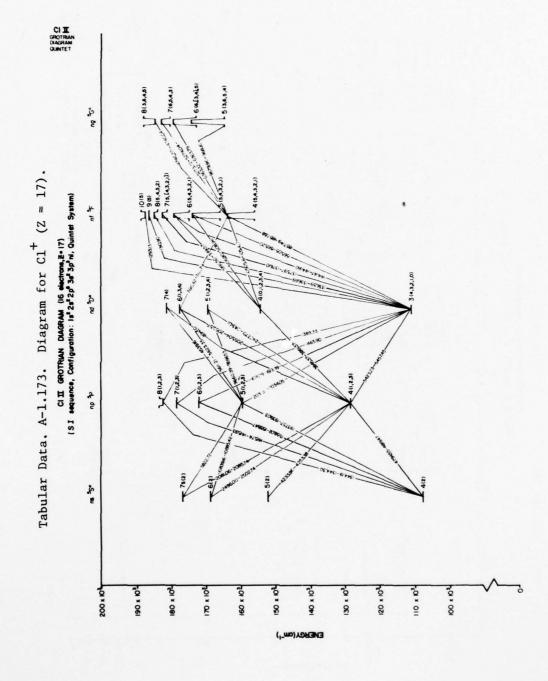






Tabular Data, A-1.172. Diagram for Cl⁺ (Z = 17). CI ENERGY LEVELS (16 electrons, Z=17)





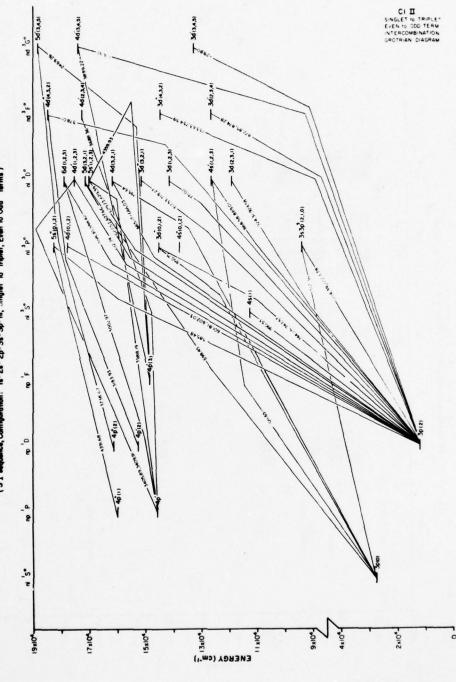
| 123,000 to the control of the con - Energy Levels Com" 8308974 8308974 8308973 83089.73 7446086 7446082 7446082 7446080 7984338 T 6(6(3,4)5) 79843,75 \$ 187628.37 (10) 186080.20 (10) 1861.330 (2) (10) 1827.320 (2) (10) 1787.134 (10) 1787.134 (10) 1787.134 (10) 1787.134 (10) Tabular Data. A-1.174. Diagram for $C1^+$ (Z = 17). 17419402 174193.79 174193.06 174192.80 (64.346) (64.3429) (64.3339) (64.3348) (64.3302) CI II ENERGY LEVELS (16 electrons, Z = 17)
(SI sequence, Configuration: 1s*2s*2p*3s*3p*n, Quintet System) COPES n1 = 3p²(*S°) n'(* = 3p³(*D°) n'f = 3p³(*P°) 1030428 1030312 1029772 102964 181515.18 — 7(4) 17726823 — 6(1,3,4) 17726823 — 6(1,3,4) 69800.79 69800.96 69800.47 69800.20 18227426 18227022 U 8(14.3) 17851473 U 7(12.3) 17850436 U 7(12.3) 15946466 - 5(1,2,3) 72063.64 172052.10 172045.05 — 6 (1,2,3) 8 15223491 -- 5(2) 16867436 -- 6(2) 107879,86 - 4(2) 17666014 - 7(2) \$ 2 190 x 103 180 x 103 170 x 103 40 x 104 30 x 10 20 x 103 110 x 103 200 x 103 160 x 103 00 : 10

CIE

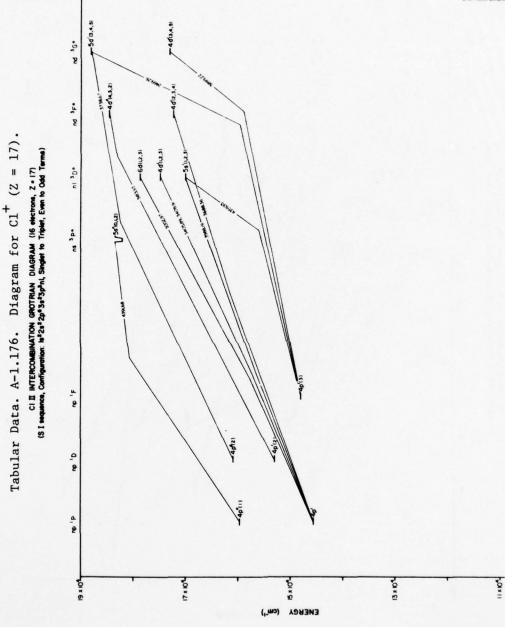
Tabular Data. A-1.175. Diagram for Cl (Z = 17).

CL INTERCOMBNATION GROTRLAN DAGRAM (16 electrons, Z=17)

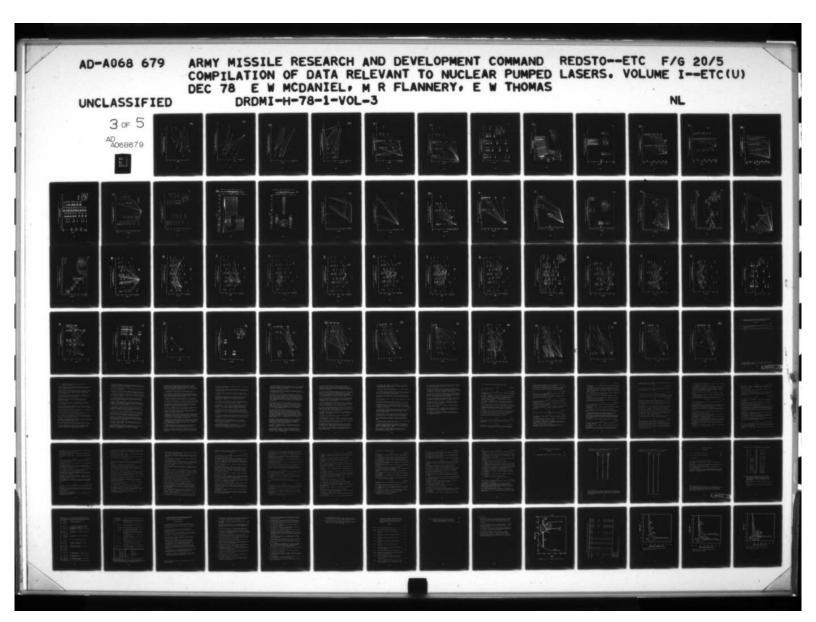
(SI sequence, Configuration: 1s² 2s² 2p³ 3s² 3p² nl, Singlet to Tuplet, Even to Odd Terms)

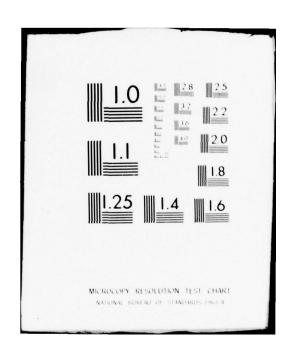


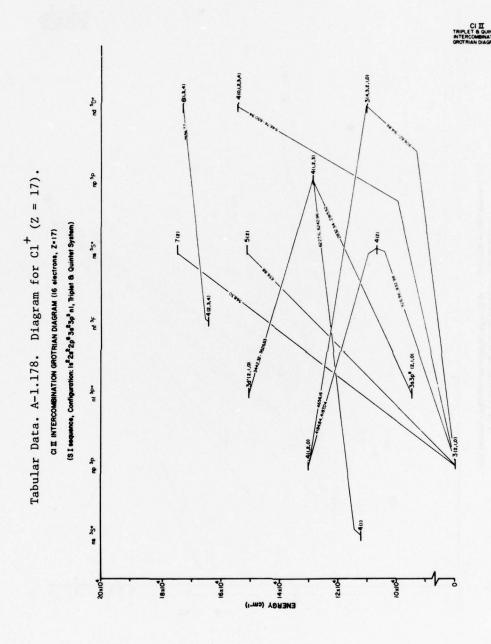
SINGLET TO TRIPLET even to odd terms INTERCOMBINATION GROTRIAN DIAGRAM

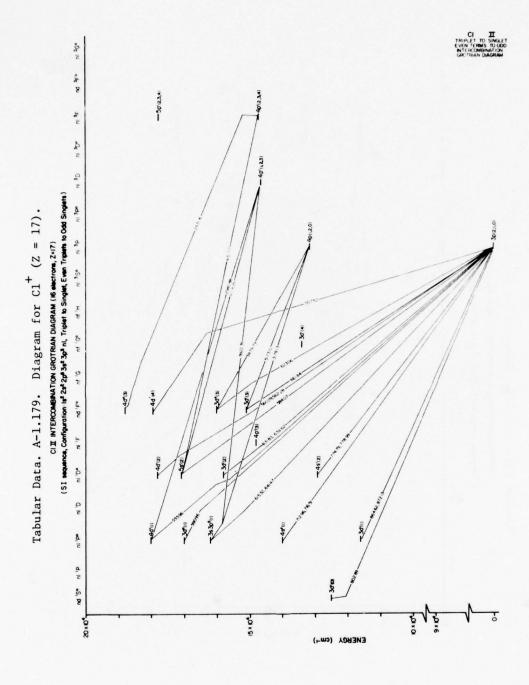


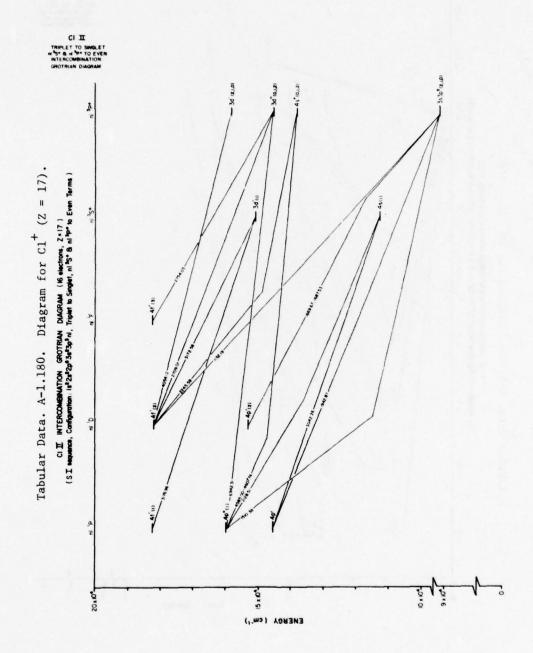
Tabular Data. A-1.177. Diagram for Cl^+ (Z = 17). CI II INTERCOMBINATION GROTRIAN DIAGRAM (16 electrons, Z = 17) (S I sequence, Configuration: $ls^2 2s^2 2p^2 3s^2 3p^2 n_1$, Singlet to Triplet, Odd to Even Terms) 11 3E 20 og, pu ed, pu , D. -d, 10 og iS. 17 x 104 13 x 104 IIx 10. ENERGY (cm-1)

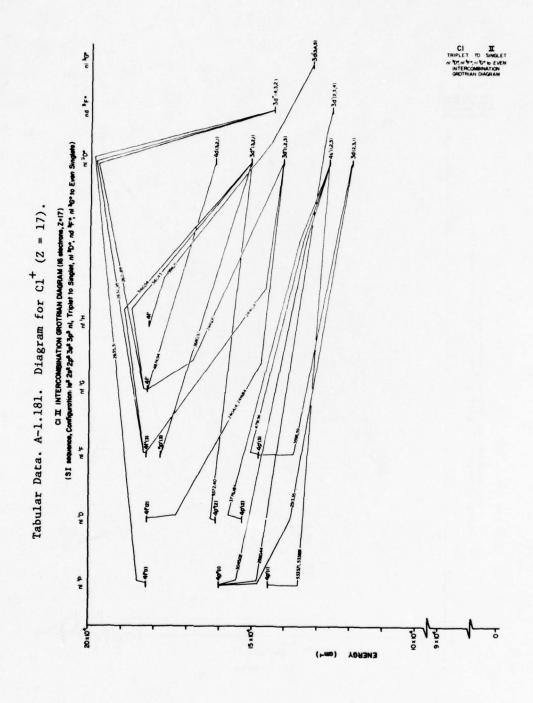


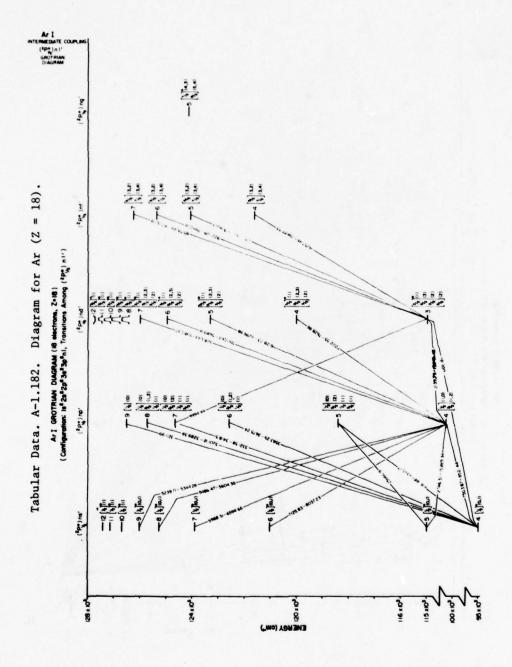


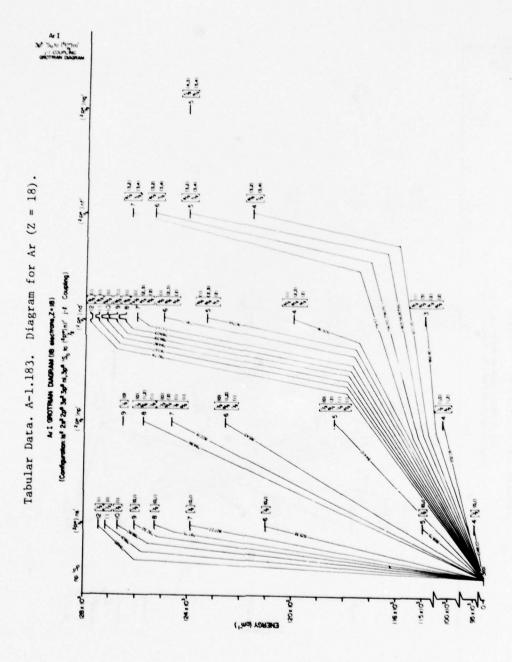


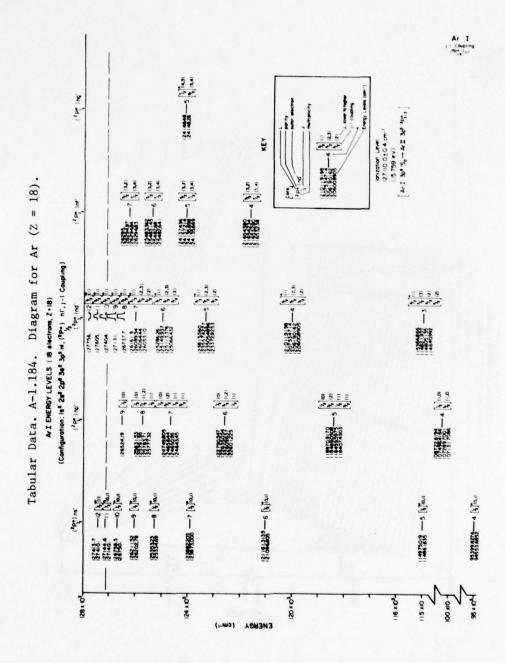


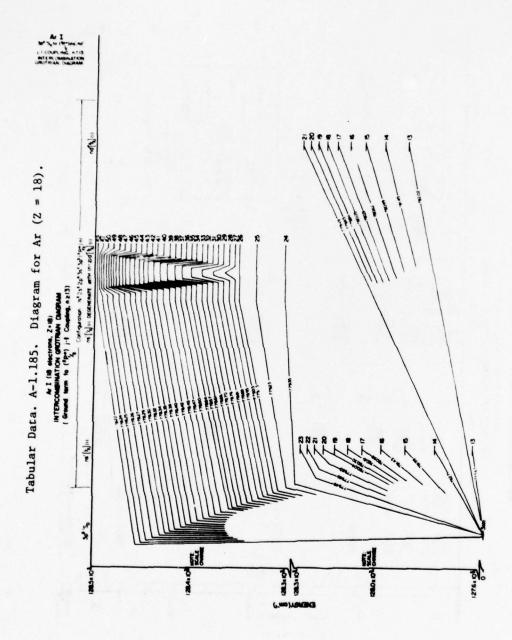




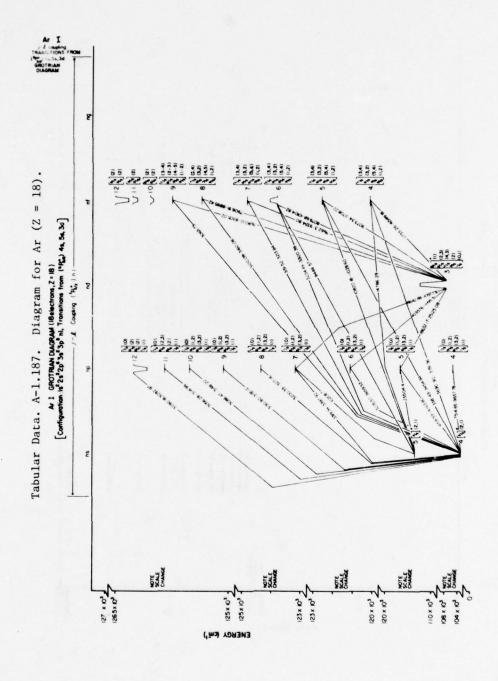


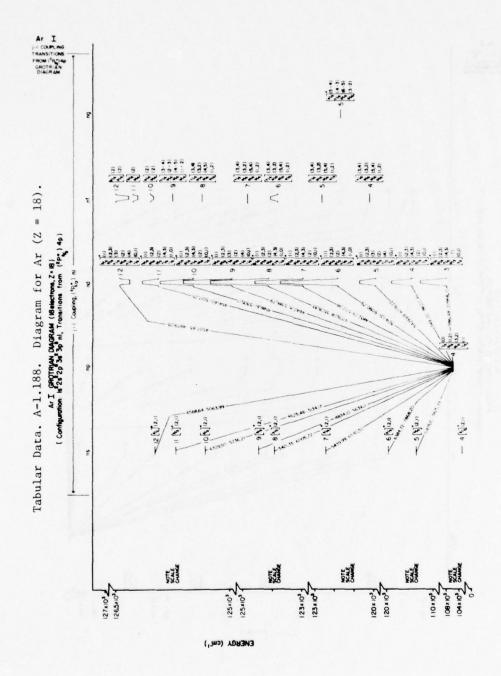


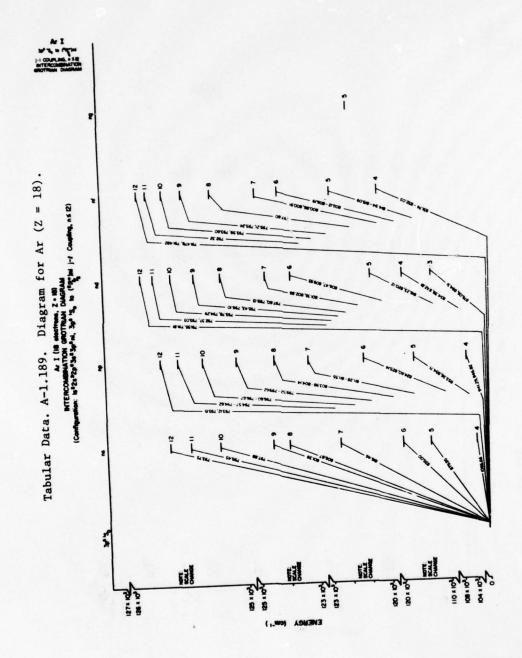


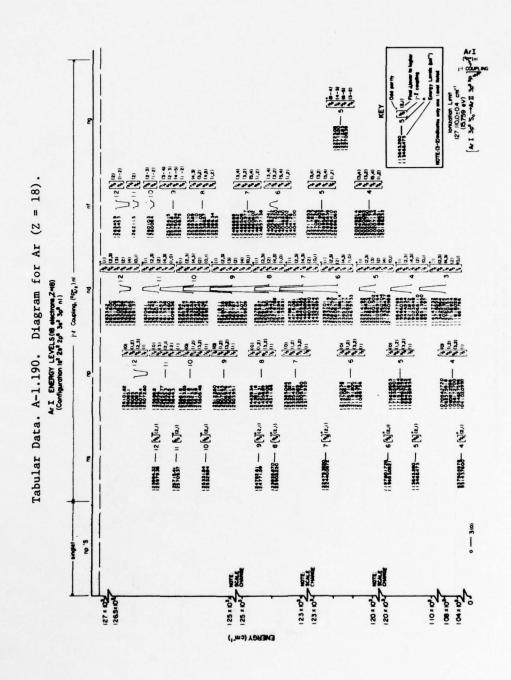


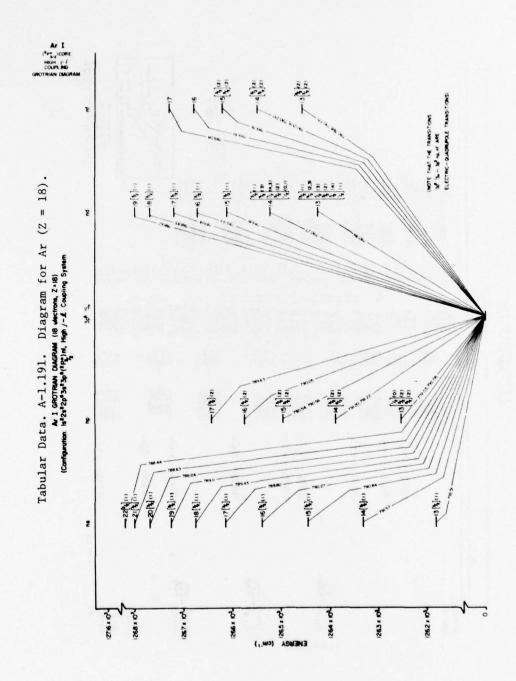
Tabular Data. A-1.186. Diagram for Ar (Z = 18). At ENERGY LEVELS (18 electrons, 2.18) (Configuration is 2st 2st 3st 3pt (1 Pr 1) ii, (1 Pr 1) iii, (1 Pr 1) iii, (1 Pr 1 Pr 1 Couping, ii 23) -61—262821 Grand Sassoy Sure 285.0



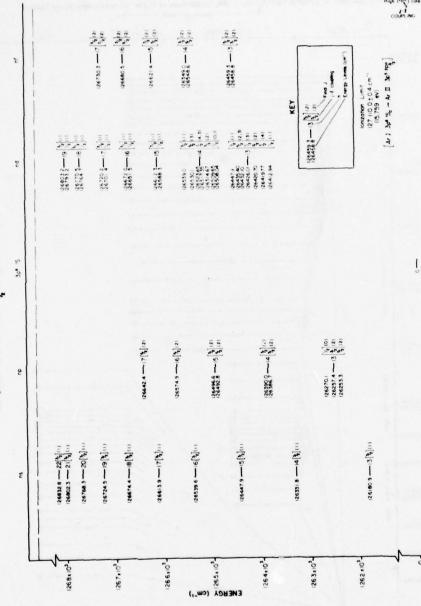




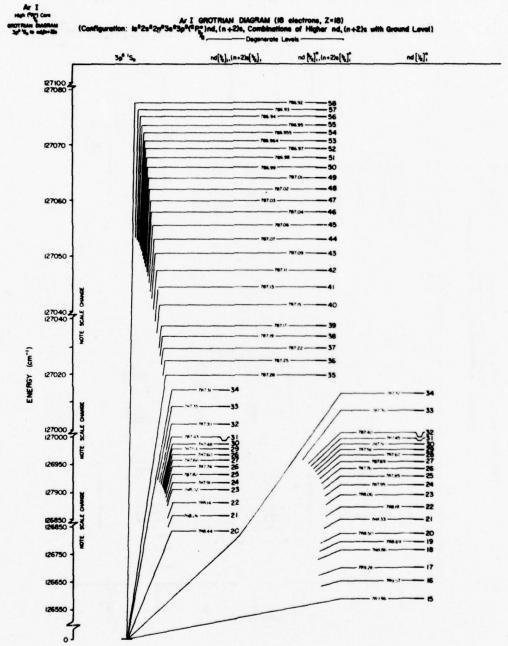




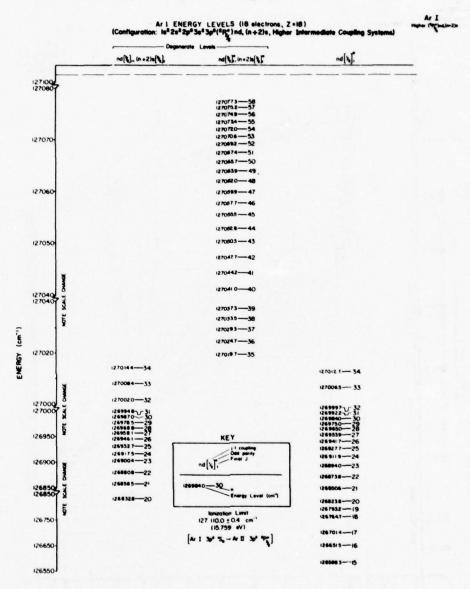
Tabular Data. A-1.192. Diagram for Ar (Z=18). Ar I ENERGY LEVELS (18 electrons, Z*18) (Configuration: N*23*20*38*39* $(^{2}_{1})_{1}$, Hop $_{1}$ -1 Coupling System)

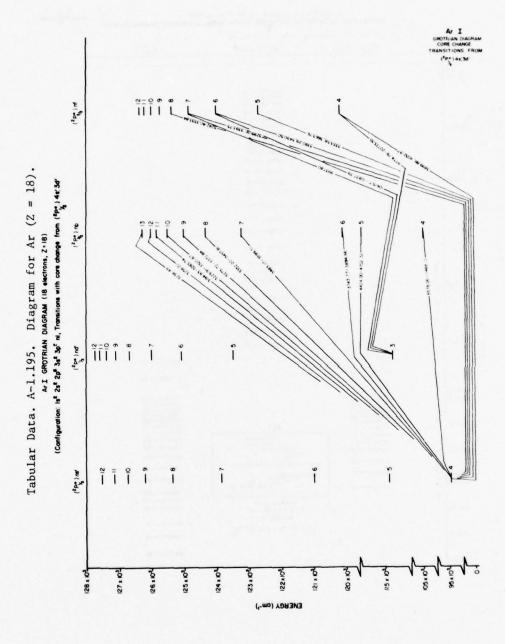


Tabular Data. A-1.193. Diagram for Ar (Z = 18).



Tabular Data. A-1.194. Diagram for Ar (Z = 18).





Tabular Data. A-1.196. Diagram for Ar (Z = 18).

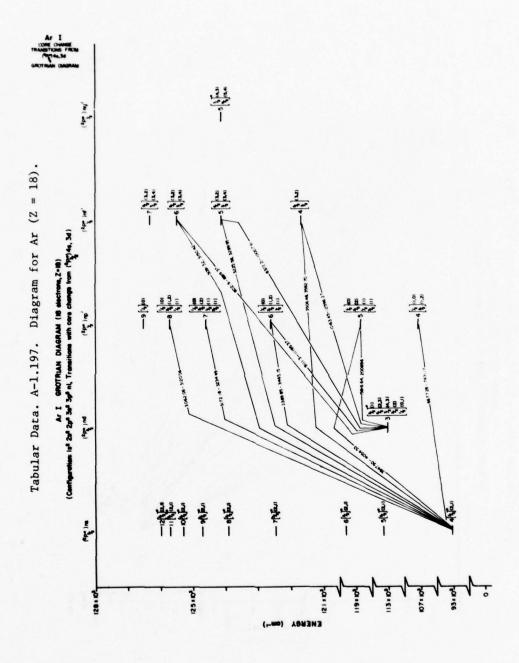
At I GROTHUM Buschul (18 deciron, Z-18)

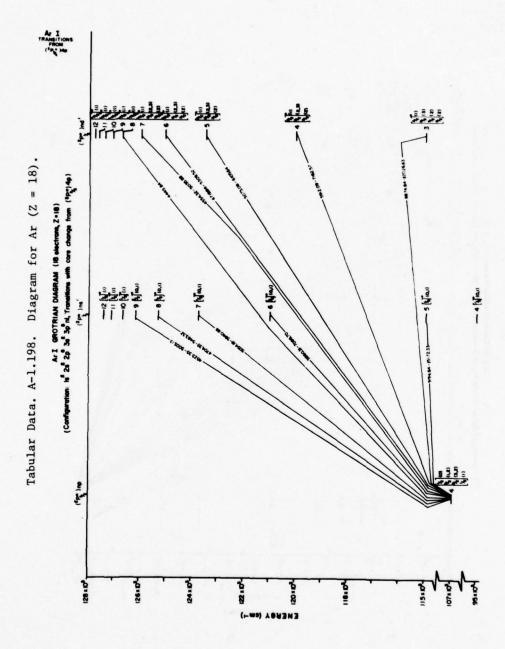
(Configuration 18 2s 2g 3s 3g 4 th Transition with core change from (Pp.) 4)

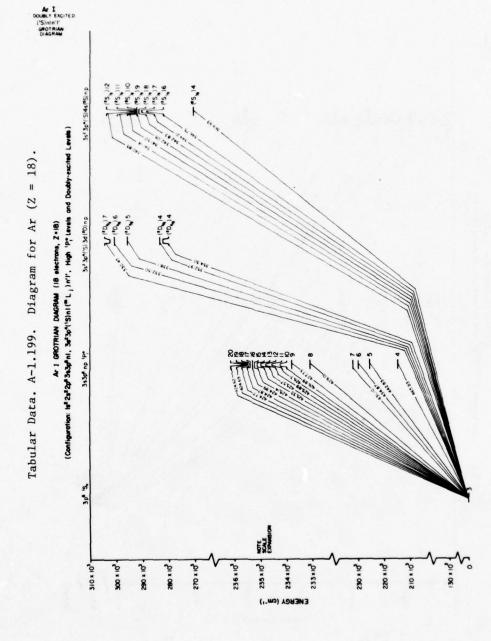
(-15, line)

(-15,

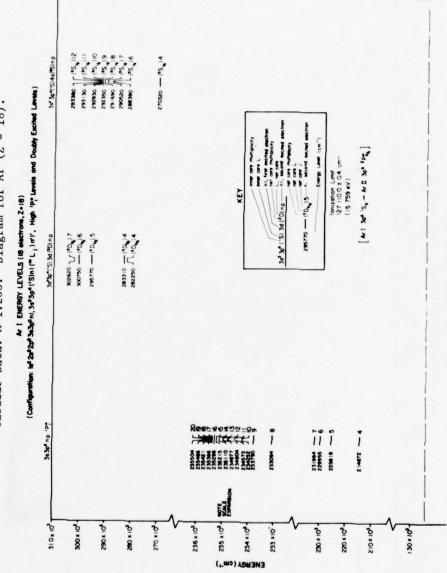
122 . 10

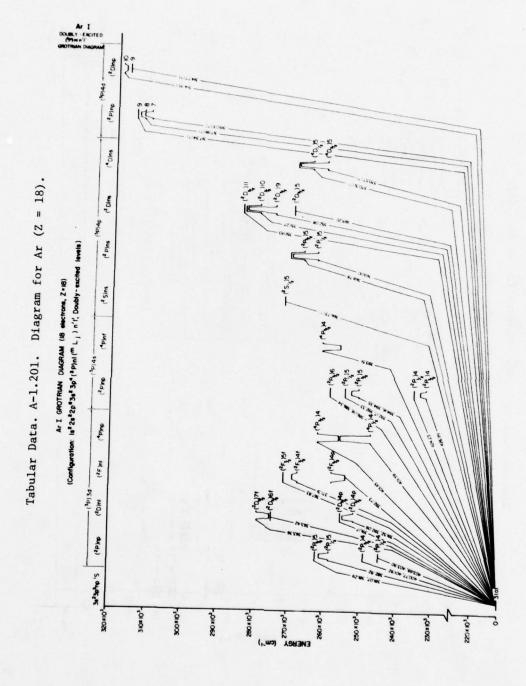






Tabular Data. A-1.200. Diagram for Ar (Z = 18).

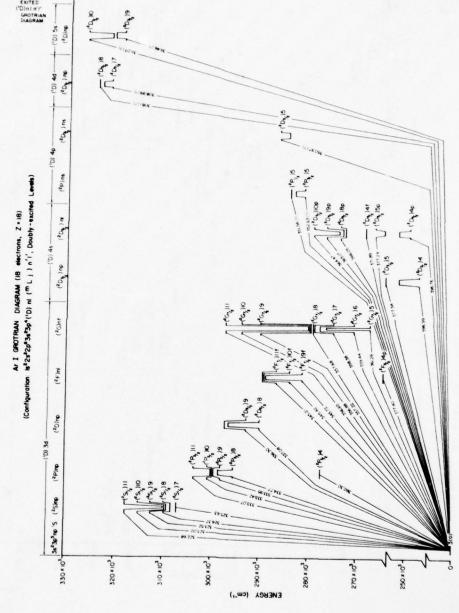




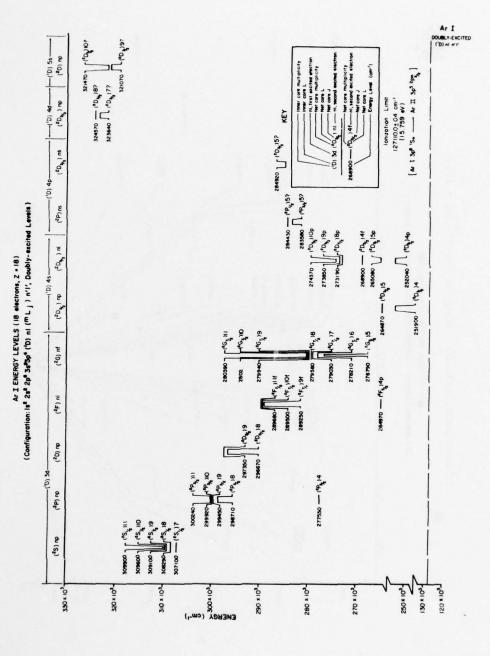
Tabular Data. A-1.202. Diagram for Ar (Z = 18).

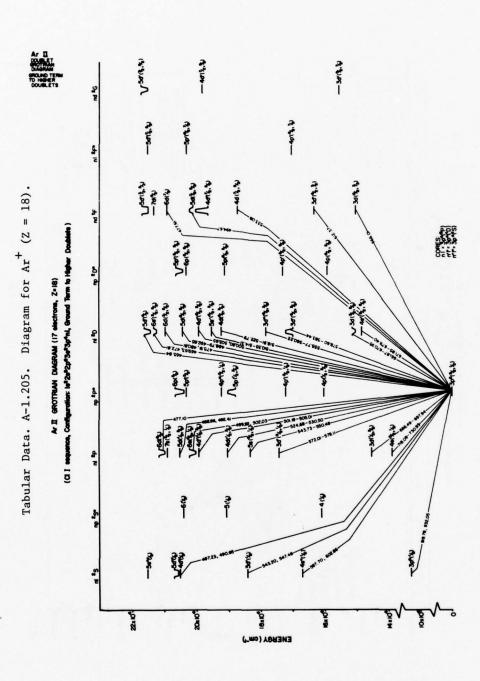
[Ar I 30° 15, - Ar II 30° 49. 315120 - 97 314490 - 97 313450 - 77 FD 18 su (0₂) Ar I ENERGY LEVELS (18 electrons, Z = i8) (Configuration: is 2 2s 2 2p 3 3p 4 (P) ii (m L $_j$) n'f, Doubly-excited levels) (20 ml Pare 320110 -01×082 300×103-310×10-

Tabular Data. A-1.203. Diagram for Ar (Z = 18).

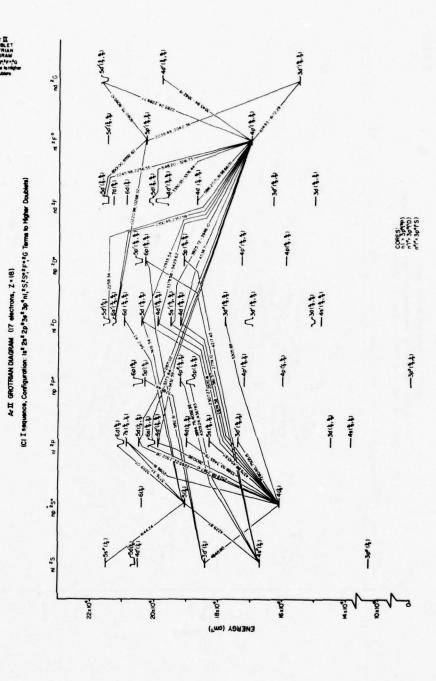


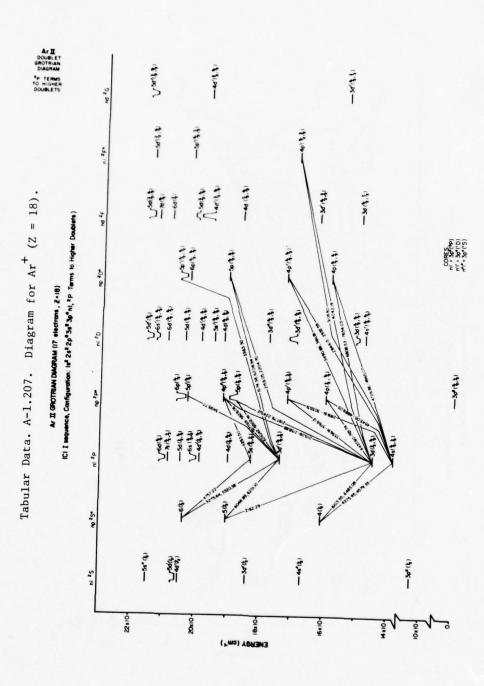
Tabular Data. A-1.204. Diagram for Ar (Z = 18).

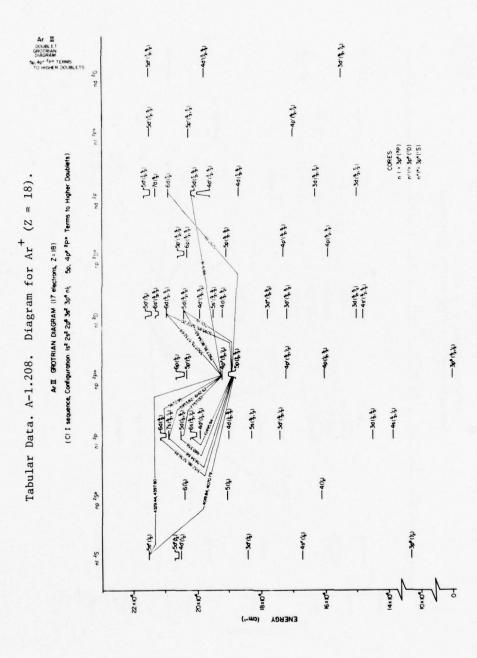


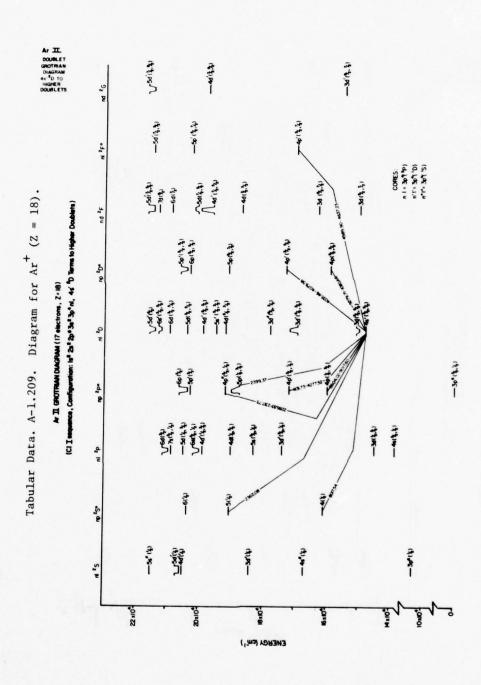


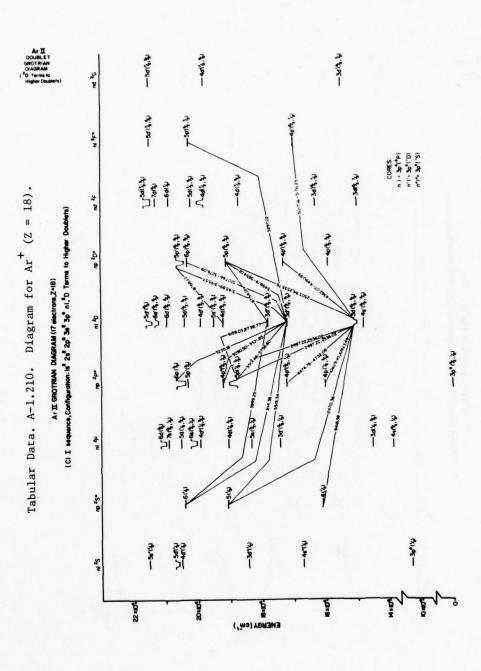
Tabular Data. A-1.206. Diagram for Ar^+ (Z = 18).

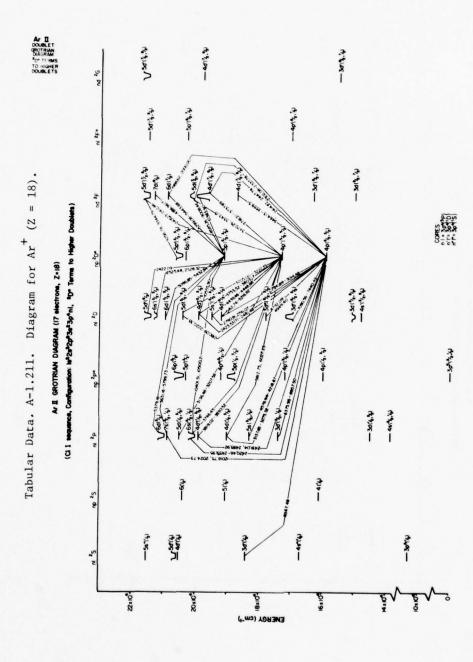


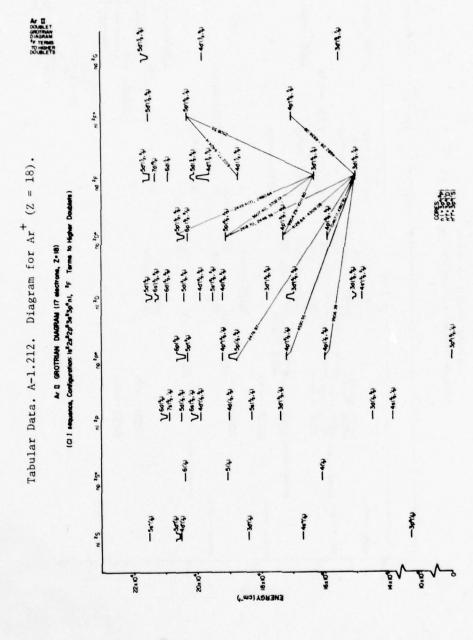




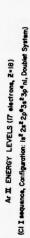


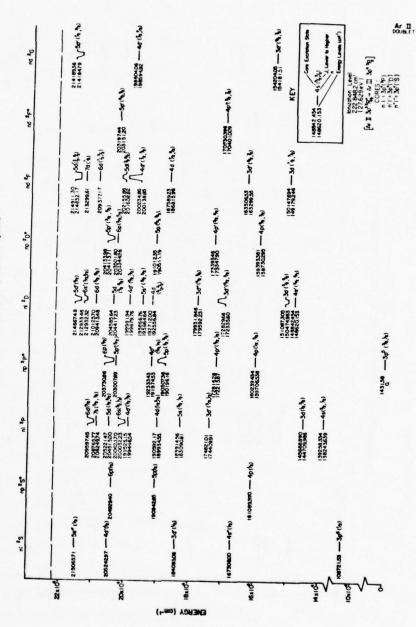




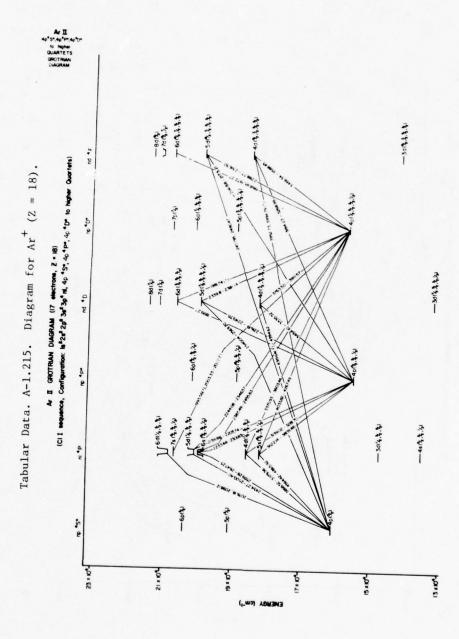


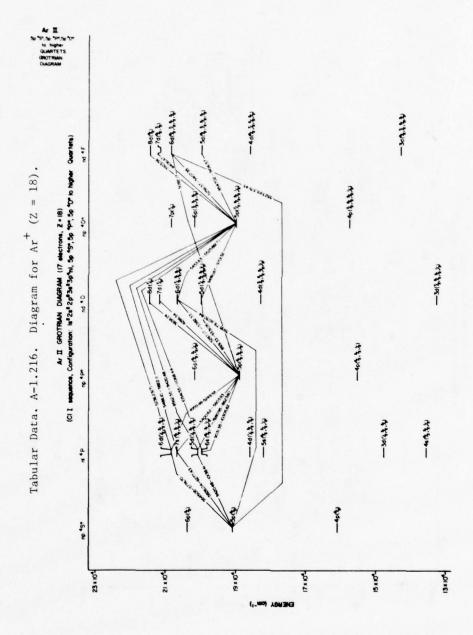
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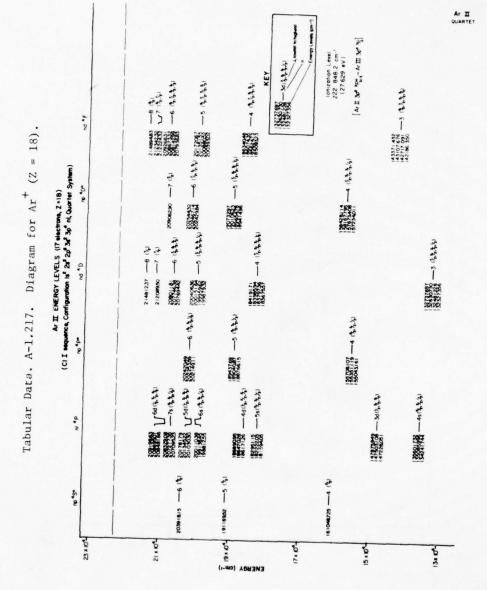


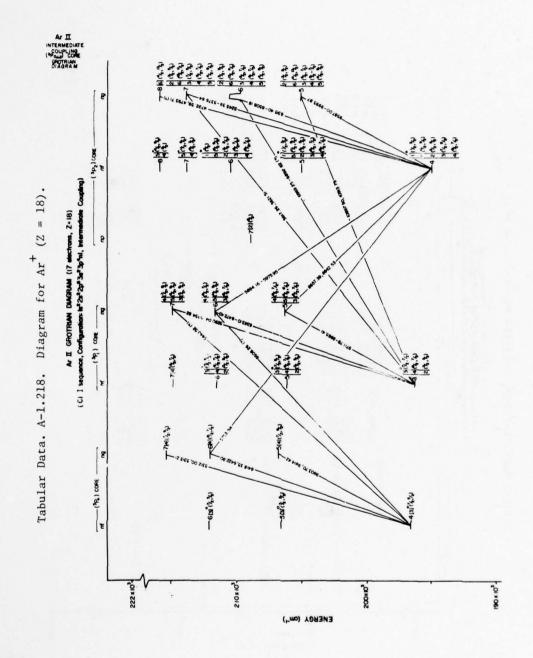


- 644.A.A. -Saft. 1.1 Tabular Data. A-1.214. Diagram for Ar^+ (Z = 18). (CLT sequence, Configuration: Inf2af2gf3af3gfM, Forestions Among Lowest Quarter Levels) 1,04 Ar II GROTPLAN DIAGRAM (17 electrons, Z = 18) 43.05-Vessian Lagan Vessian \$ 2 6 21 10

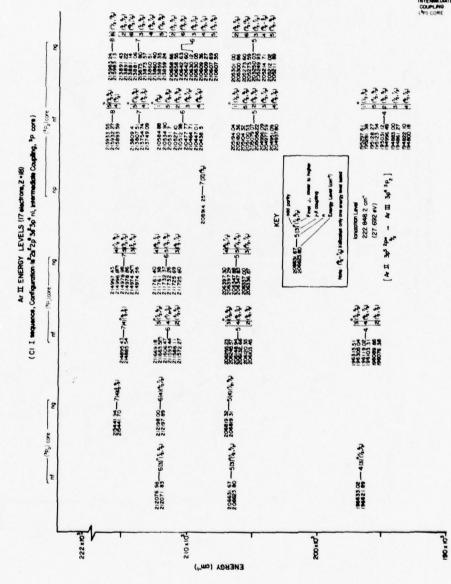


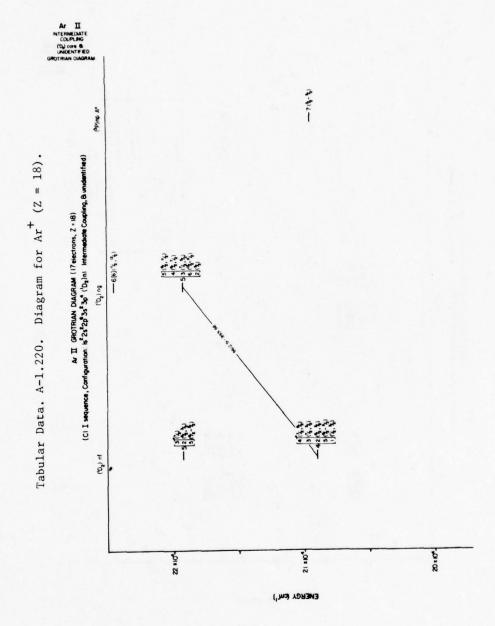




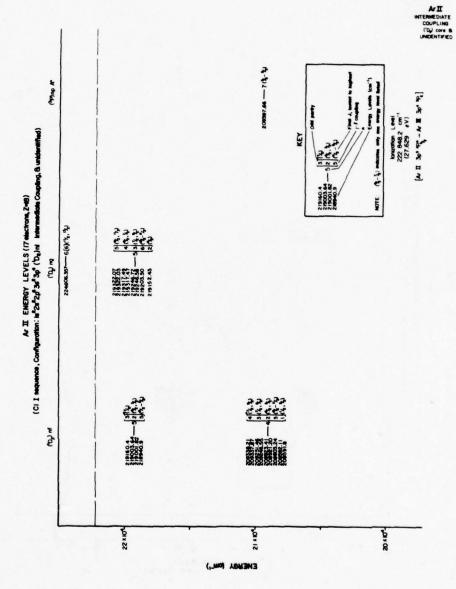


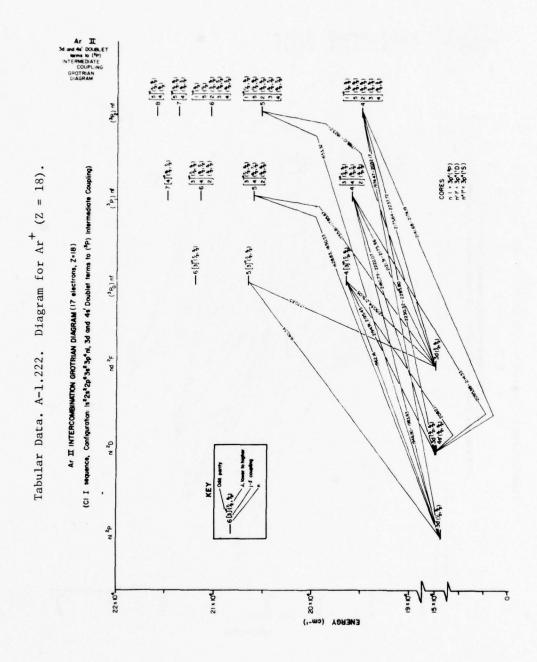
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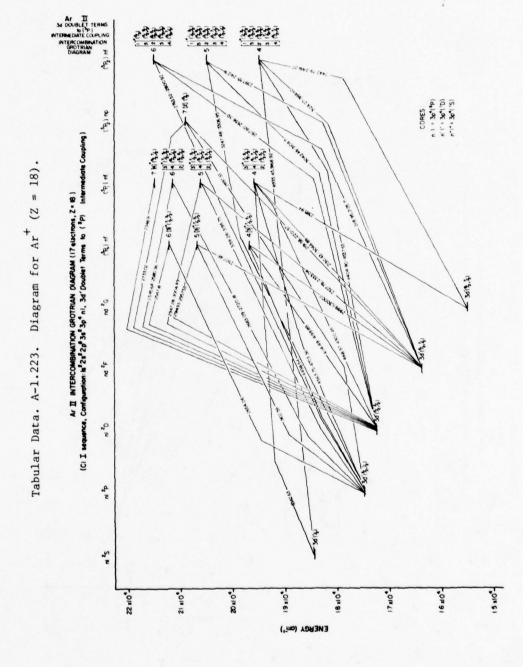


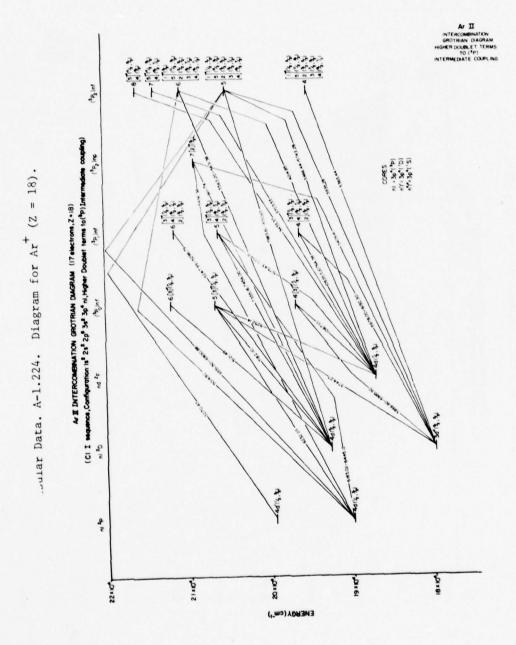


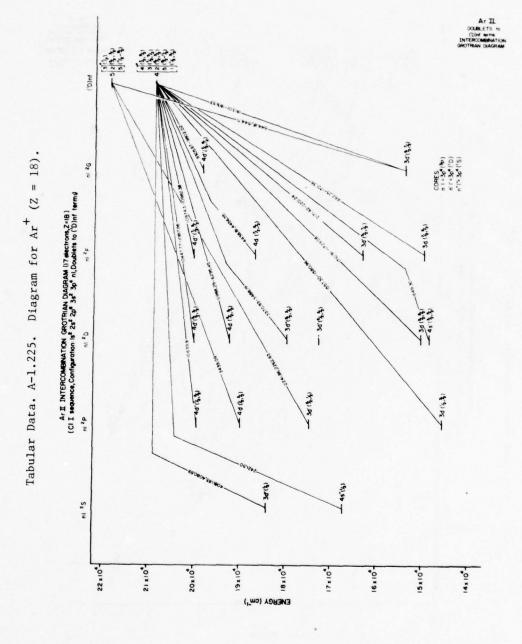
Tabular Data. A-1.221. Diagram for Ar $^+$ (Z = 18).



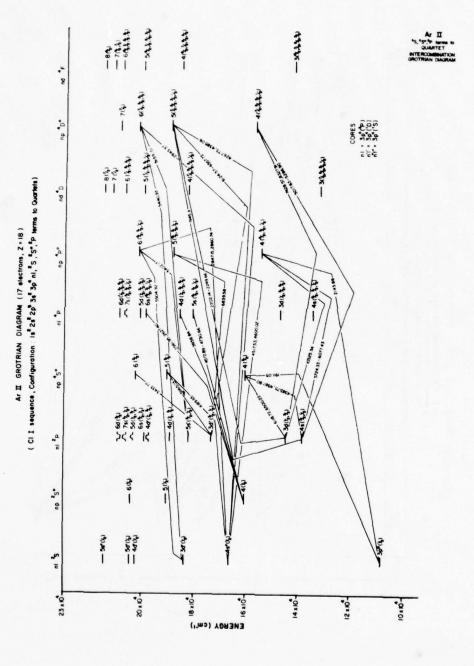


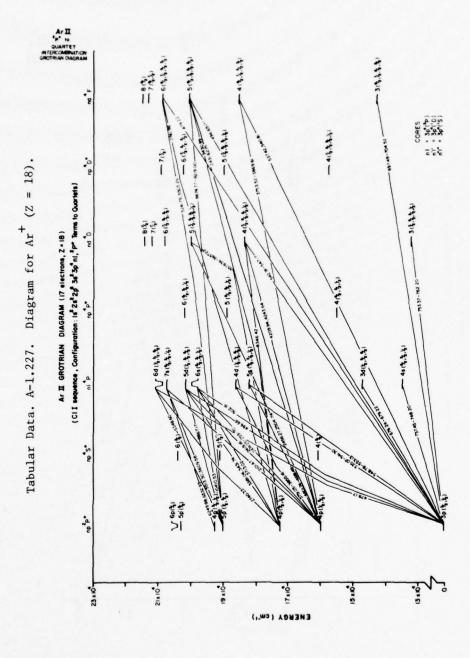




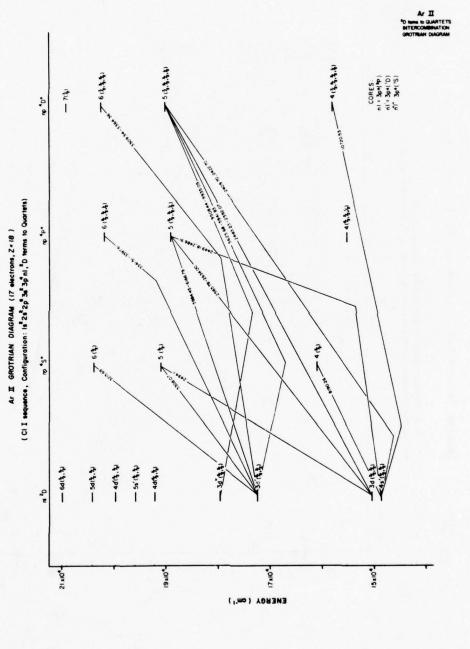


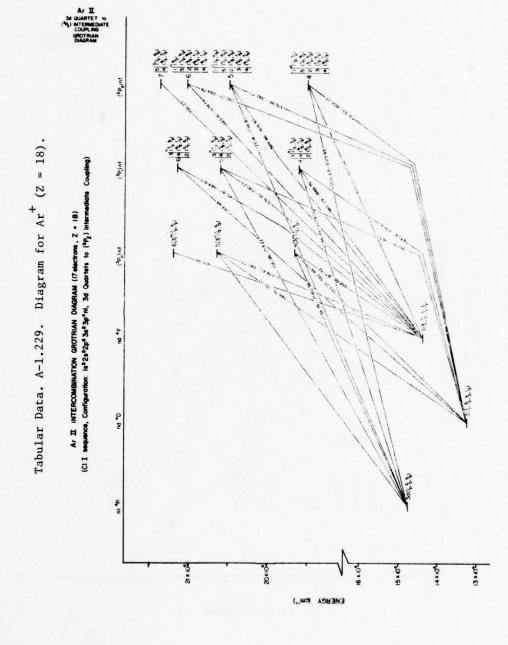
Tabular Data. A-1.226. Diagram for Ar^+ (Z = 18).



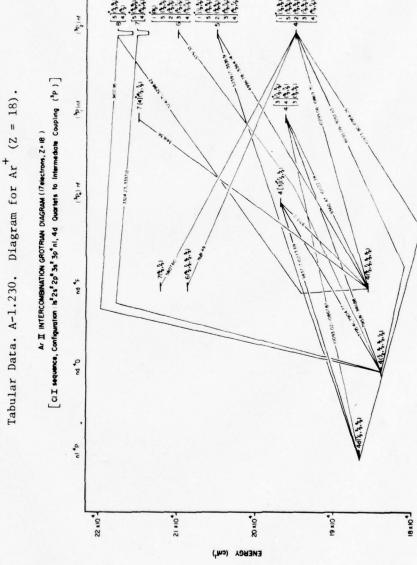


Tabular Data. A-1.228. Diagram for Ar (Z = 18).









A-2. REFERENCES ON ATOMIC ENERGY LEVELS, SPECTRAL LINES, LIFTIMES, OSCILLATOR STRENGTHS, AND TRANSITION PROBABILITIES*

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^{*}For data on radiative lifetimes of the rare gas atoms and molecules, see pages 194-212 of Vol. I.

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A-2.2. References on Specific Atoms of Relevance Here

H Z = 1 1 electron

See the general references.

He Z = 2 2 electrons

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 B^+ Z = 5 4 electrons

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Z = 6 6 electrons

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 C^{+} Z = 6 5 electrons

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N Z = 7 7 electrons

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Z = 8 8 electrons

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 0^+ Z = 8 7 electrons

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Z = 9 9 electrons

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Z = 9 8 electrons

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Ne Z = 10 10 electrons

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Ne⁺ Z = 10 9 electrons

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A1 Z = 13 13 electrons

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Z = 16

16 electrons

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s+

Z = 16

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C1 Z = 17 17 electrons

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Z = 17 16 electrons

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Ar Z = 18 18 electrons

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Ar+

Z = 18

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Z = 36

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Xe

T+

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A-3. POLARIZABILITIES AND MULTIPOLE MOMENTS

CONTENTS

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A-3.1.	Recommended Values for the Polarizabilities of Ground	
	State Atoms	• 1156

Tabulated Data. A-3.1. Recommended values for the polarizabilities of ground state atoms in units of $10^{-24}~{\rm cm}^3$.*

Estimated		
accuracy (%)	Atom	Average polarizability
"Exact"	Н	0.666793
0.5	He	0.204956
	Li	24.3
2	Be B	5.60
2	C	3.03
•	N	1.76
2	o O	1.10
1	F	0.802
;	Ne Ne	0.557 0.395
2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	Na Na	23.6
,	Mg	10.6
,	Al	8.34
,	Si	5.38
,	P	3.63
2	S	2.90
2	CI	2.18
0.5	Ar	1.64
2	K	43.4
8	Ca	25.0
50	Sc	16.9
50	Ti	13.6
50	v	11.4
50	Cr	6.8
50	Mn	8.6
50	Fe	7.5
50	Co	6.8
50	Ni	6.5
50	Cu	6.1
2	Zn	7.08
2	Ga	8.12
2 2 2 2	Ge	6.07
2	As	4.31
	Se	3.77
2	Br	3.05
0.5	Kr	2.48
2	Rb	47.3
8	Sr	27.6
50	Y	22
50	Zr	18

^{*}From T. M. Miller and B. Bederson, "Atomic and Molecular Polarizabilities-A Review of Recent Advances," in "Advances in Atomic and Molecular Physics" (D. R. Bates and B. Bederson, Eds.), Vol. 13, Academic Press, New York (1977).

Tabulated Data A-3.1. Recommended values for the polarizabilities of ground states atoms in units of $10^{-24}~{\rm cm}^3$ (Continued).

Estimated		
accuracy		Average
(".)	Atom	polarizability
50	Nb	14
50		13
50	Мо	
50	Tc Ru	10.0
50	Rh	8.6
50	Pd	7.6
50	Ag	6.9
50	Cd	6.0
50	In	4.5
50	Sn	4.4
50	Sb	4.0
50	Te	3.9
50	i	3.9
0.5	Xe	4.04
2	Cs	59.6
8	Ba	39.7
50	La	37
50	Ce	36
50	Pr	34
50	Nd	32
50	Pm	30
50	Sm	29
50	Eu	27
50	Gd	26
50	ТЬ	25
50	Dy	25
50	Ho	23
50	Er	23
50	Tm	22
50	Yb	22
50	Lu	20
50	Hſ	15
50	Ta	13
50	w	10
50	Re	9
50	Os	8
50	lr .	7
50	Pt	6.3
50	Au	5.7
50	Hg	5.1
50	TI	3.5
50	Pb	3.7
50	Bi	4.0
50	Po	4.6
50	At	5.1
50	Rn	6.3
50	Fr	67
50	Ra	46
50	Ac	53
50	Th	50
50	Pa	48
50	U	46
50	Np	45
50	Pu	43
50	Am	41
50	Cm	40
50	Bk	39
50	Ct	38
50	Es	36
50	Fm	35
50	Md	34
50	No	33
50	Lw	32

A-4. ELECTRON AFFINITIES*

CONTENTS

A-4.1.	Electron Affinities of Atoms	1161
A-4.2.	Electron Affinities of Molecules	1162
A-4. Re	eferences:	
A. P. M.	Baede, Adv. Chem. Phys. <u>30</u> , 463 (1975).	
R. N. Co 2023 (19	ompton, P. W. Reinhardt, and C. D. Cooper, J. Chem. Phys. 178).	<u>68</u> ,

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For discussions of the difference between electron affinities and vertical detachment energies for molecules, see H.S.W. Massey, "Negative Ions," (Third Edition) Cambridge University Press, Cambridge (1976), pg. 166 and E. W. McDaniel, "Collision Phenomena in Ionized Gases," Wiley, New York (1964), pg. 379.

Tabular Data. A-4.1. Electron Affinities of Atoms (in eV).

Не	< 0	Ag	1.303 (7)
Ne	< 0	A1	0.46 (3)
Ar	< 0	В	0.28 (1)
Kr	< 0	С	1.268 (5)
Xe	< 0	Cd <	0
		Cu	1.226 (10)
F	3.399 (3)	D*	0.757 ± 0.005
C1	3.615 (4)	Н	0.7542 (3)
Br	3.364 (4)	Hg <	0
I	3.061 (4)	In	0.30 (15)
		N -	0.07 (8)
Li	0.620 (7)	0	1.462 (3)
Na	0.546 (5)	P	0.743 (10)
K	0.5012(5)	S	2.0772 (5)
Rb	0.4860(5)	Se	2.0206 (3)
Cs	$0.4715 \binom{5}{20}$	Te	1.9708 (3)
Fe [†]	0.164 ± 0.035	U	unmeasured at this date

Note: Unless otherwise indicated, the data here are recommended values from Table 10 in the critical review:
H. Hotop and W. C. Lineberger, "Binding Energies in Atomic Negative Ions," Jour. Phys. Chem. Ref. Data 4, 539-576 (1975).

^{*}K. E. McCulloh and J. A. Walker, Chem. Phys. Lett. <u>25</u>, 439 (1974).

[†]P. C. Engelking and W. C. Lineberger, Phys. Rev. <u>A</u> <u>19</u>, 149 (1979).

Tabular Data. A-4.2. Electron Affinities of Molecules (in eV).

F ₂	3.08 ± 0.1	
Cl 2	2.38 ± 0.1	W. A. Chupka, J. Berkowitz, and D. Gutman.
Br ₂	2.51 ± 0.1	J. Chem. Phys. <u>55</u> , 2724 (1971).
12	2.58 <u>+</u> 0.1	
IBr	2.7 <u>+</u> 0.2	
ICL	1.43	J. Jortner and U. Sokolov, Nature 190, 1003 (1961).
L1CL	0.61 ± 0.02	J. L. Carlsten, J. R. Peterson, and W. C. Lineberger, Chem. Phys. Lett. 37, 5 (1976).
Fe0	1.492 <u>+</u> 0.020	P. C. Engelking and W. C. Lineberger, J. Chem. Phys. $\underline{66}$, 5054 (1977).
	0.381 ± 0.014	P. C. Engelking and W. C. Lineberger, J. Chem. Phys. $\underline{65}$, 4323 (1976).
NH(a¹∆)	1.960 ± 0.010	
PO	1.092 ± 0.010	P. F. Zittel and W. C. Lineberger, J. Chem. Phys. 65,
PH	1.028 ± 0.010	1236 (1976).
PH ₂	1.271 ± 0.010	
UF ₆	≥ 5.1	R. N. Compton, J. Chem. Phys. <u>66</u> , 4478 (1977).
UF ₅	4.0 ± 0.4	
CF ₃ Br	0.91 <u>+</u> 0.2	R. N. Compton, P. W. Reinhardt, and C. D. Cooper,
CF3I	1.57 ± 0.2	J. Chem. Phys. <u>68</u> , 4360 (1978).
SF ₆	0.46 ± 0.2	R. N. Compton, P. W. Reinhardt, and C. D. Cooper,
SeF ₆	2.9 ± 0.2	J. Chem. Phys. 68, 2023 (1978).
TeF ₆	3.3 ± 0.2	
SF5	2.71 ± 0.2	
SF ₄	0.78 ± 0.2	
SF ₃	3.07 ± 0.2	
СН	1.238 ± 0.008	A. Kasdan, E. Herbst and W. C. Lineberger, Chem. Phys. Lett. 31, 78 (1975).
NH ₂	0.779 <u>+</u> 0.037	R. J. Celotta, R. A. Bennett and J. L. Hall, J. Chem. Phys. <u>60</u> , 1740 (1974).
СНЗО	1.570 ± 0.022	
CD30	1.552 + 0.022	P. C. Engelking, G. B. Ellison, and W. C. Lineberger, J. Chem. Phys. 69, 1826 (1978).
CH3S	1.882 ± 0.024	5. Gien. Tilye. <u>07</u> , 1020 (1770).

Tabular Data. A-4.2. Electron Affinities of Molecules (in eV) (Continued).

CN	3.82	+ 0.02			Chupka and T. A. Walter, J. Chem.	
			Phys	. <u>50</u> , 1497 (196	99).	
С2Н	3.73		D. F	eldmann, Z. Nat	urforsch. Teil A <u>25</u> , 621 (1970).	
c_2	3.54					
ОН	1.8255	5 ± 0.002		otop, R. A. Ber . <u>58</u> , 2373 (197	nett and W. C. Lineberger, J. Chem.	
NO	0.024	+ 0.010 - 0.005			Celotta, J. L. Hall, J. Levine and Rev. A <u>6</u> , 607 (1972).	
02	0.440	<u>+</u> 0.008			A. Bennett, J. L. Hall, M. W. Siegel . Rev. A <u>6</u> , 631 (1972).	
CH ₂	0.21	<u>+</u> 0.03	W. C		d W. P. Reinhardt, J. Am. Chem. Soc.	
co ₂	-0.6			. Compton, P. W	Reinhardt, and C. D. Cooper, J. Chem.	
N ₂ O	0.22	<u>+</u> 0.1		. Hopper, A. C. nem. Phys. <u>65</u> ,	Wahl, R. L. C. Wu and T. O. Tiernan, 5474 (1976).	
03	2.14	<u>+</u> 0.15		Rothe, S. Y. (1975).	Tang, and G. Reck, J. Chem. Phys. <u>62</u> ,	
NO ₂	2.36	<u>+</u> 0.1		erbst, T. A. Pa . <u>61</u> , 1300 (197	tterson, and W. C. Lineberger, J. Chem. 4).	
во2	4.07	<u>+</u> 0.2	D. E	. Jensen, Trans	. Faraday Soc. <u>65</u> , 2123 (1969).	
co ₃	2.9	<u>+</u> 0.3		. Moseley, P. C. Cosby and J. R. Peterson, J. Chem. Phys. 2512 (1976).		
HNO 3	0.57	+ 0.15	В. Р	Mathur, E. W.	Rothe, S. Y. Tang, and Kanwai Mahajan,	
NO ₃	3.68	+ 0.2		nem. Phys. <u>64</u> ,		
co ₄	1.22		J. L	. Pack and A. V	. Phelps, J. Chem. Phys. 45, 4316 (1966	
н ₂		-1.7		NCO	>2.6 + 0.4	
CH ₃		1.08		CS	<1.2	
OD		1.823 + 0.00	02	so	1.09 + 0.05	
C ₂		3.54 + 0.05		S ₂	1.663 + 0.040	
C ₂ H		3.73 + 0.05		04	negative ion detected	
SIH		1.277 + 0.00	09	SO ₂	1.097 + 0.036	
SiH ₂		1.124 + 0.03		CO3(H2O)	2.1	
2			10	3. 2.		

^{*}From the chapter "Negative Ions" by B. L. Moiseiwitsch in "Atomic Processes and Applications", P. G. Burke and B. L. Moiseiwitsch, (Eds). 314-315 (North-Holland Publishing Co., Amsterdam, 1976).

A-5. GENERAL REFERENCES ON POTENTIAL ENERGY CURVES, ELECTRONIC ENERGIES, SPECTROSCOPIC CONSTANTS AND ABSORPTION AND EMISSION SPECTRA OF EXCIMER SYSTEMS *

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A-6. POTENTIAL ENERGY CURVES, ELECTRONIC ENERGIES AND SPECTROSCOPIC CONSTANTS FOR xe_2^+ AND xe_2^* . INTERACTIONS BETWEEN LIKE AND UNLIKE PAIRS OF RAREGAS ATOMS

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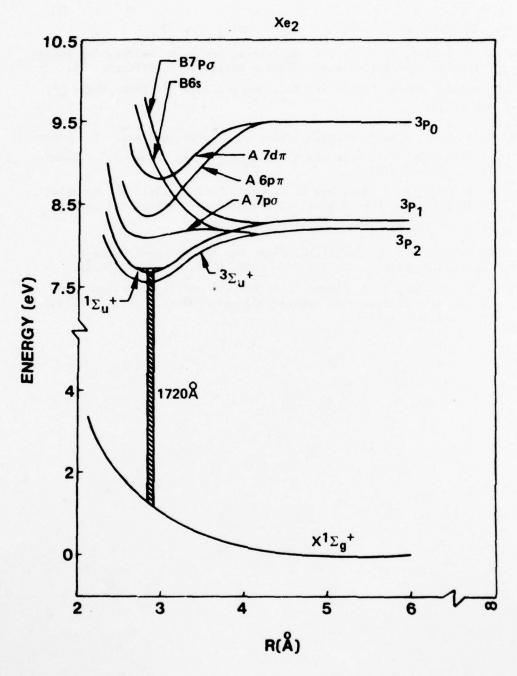
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A-6. References:

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Graphical Data. A-6.1. Electronic transition laser— Xe_2 .

Tabular Data A-6.2. Spectroscopic constants for Xe_2^+ and Xe_2^* .

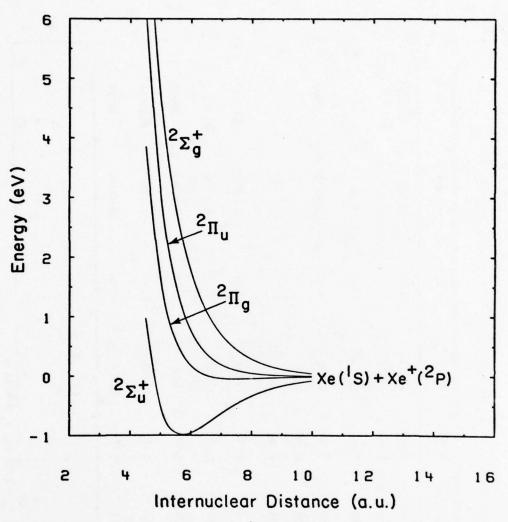
		$R_e(a_0)$	D _e (eV)	ω _e (cm ⁻¹)	we X (cm 1)	B (cm ⁻¹)	$\alpha_{\rm e}({\rm cm}^{-1})$
$xe_2 + 2r_4$	es .	5.74	0.99	122.5	0.45	0.02786	0.00011
	P	80.9	1.08	124			
	υ	5.84	1.04	125			
$(1/2)^{d}_{u}$	æ	5.82	0.70	110.4	0.53	0.02704	0.00013
	д	6.18	0.79	112			
	U	5.91	92.0	112			
xe_2 xe_2 xe_3	a	2.67	1.00	128.3	0.62	0.02856	0,00012
$^{1}\Sigma_{\mathrm{u}}^{+}$	a	5.65	1.03	129.2	0.45	0.02868	0.00011
+ ₀ "	a	5.72	0.77	118.5	0.53	0.02800	0.00013
'o"	rd	5.73	0.78	117.3	0.59	0.02793	0.00014
J.	a	5.73	0.79	118.0	0.59	0.02796	0.00014

a Reference 1.

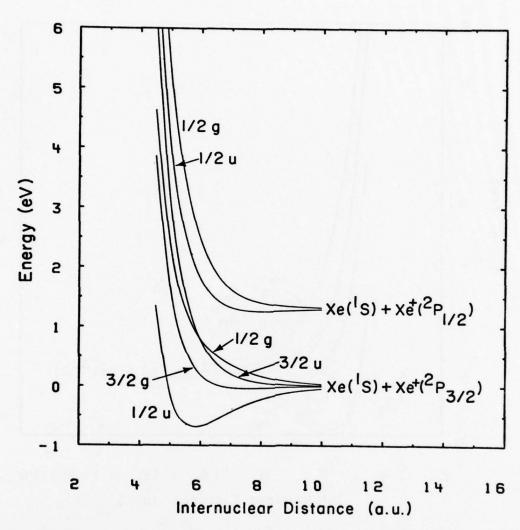
b Reference 2.

c Reference 3.

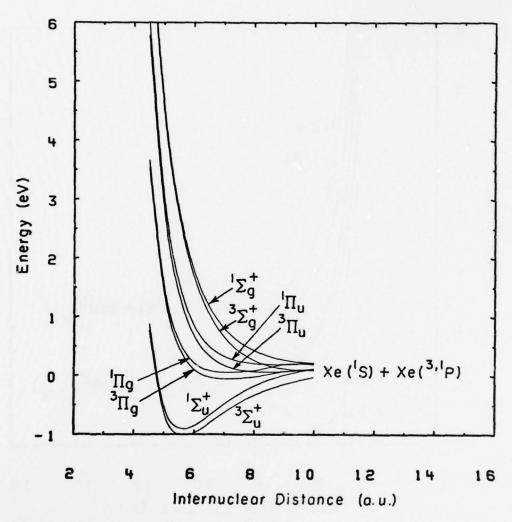
d Empirical estimate of D_o = 1.03 eV, R_e = 6.14 a_o.



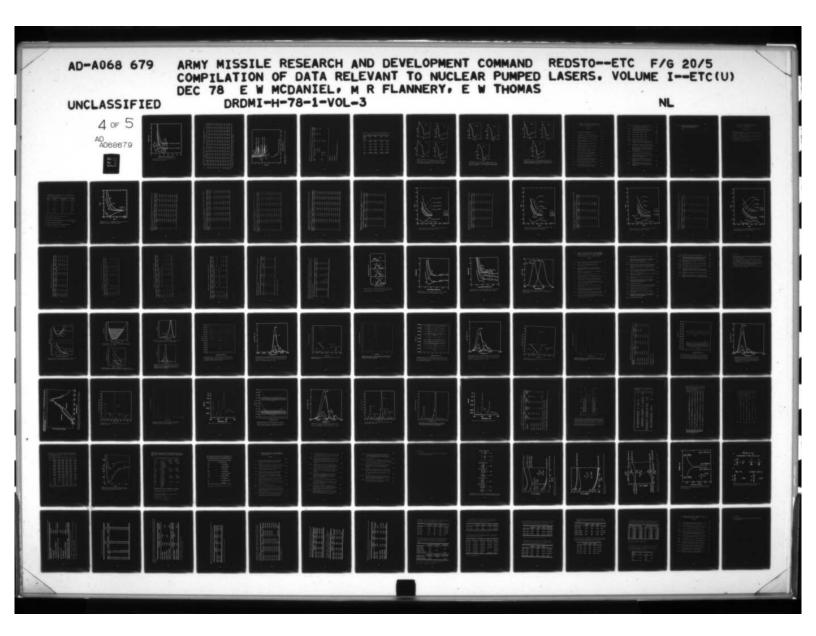
Graphical Data. A-6.3. Xe_2^+ potential energy curves without spin-orbit coupling.

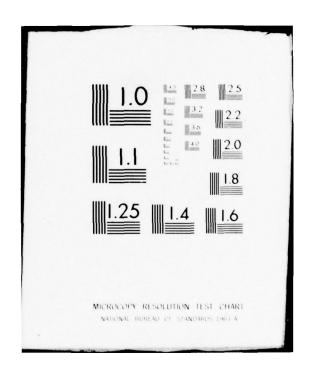


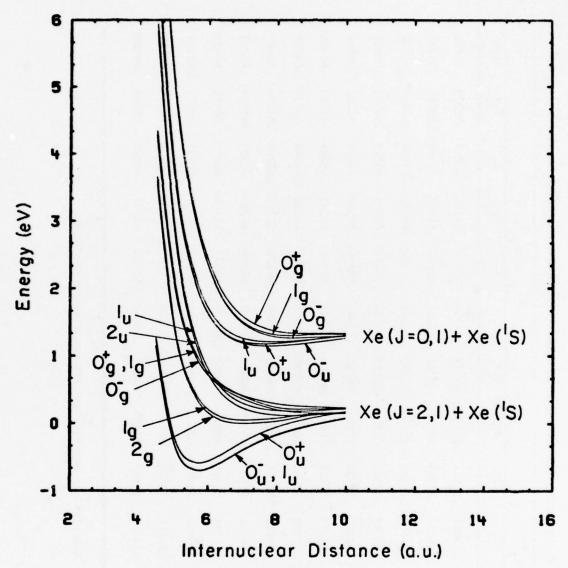
Graphical Data. A-6.4. Xe_2^+ potential energy curves including spin-orbit coupling.



Graphical Data. A-6.5. Xe_2^* potential energy curves without spin-orbit coupling.





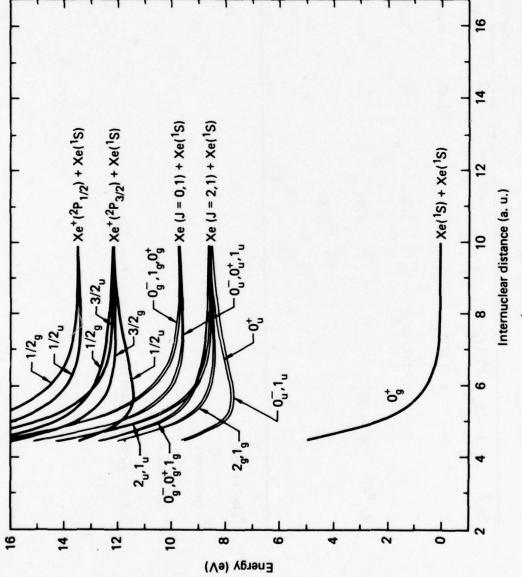


Graphical Data. A-6.6. Xe_2^* potential energy curves including spin-orbit coupling.

Tabular Data. A-6.7. Valence SCF energies of electronic states of diatomic Xeª.

	Xe ₂		×	xe ₂ ⁺					xe2	* ~			
~	12+	2 ₂ +	2 _{II} 8	2 _T	2 ₂ +	3°+	1 ₂ +	3 _π	1 8	3 _n	In u	3°+	1 ₂ +
4.50	.81444 .53110	.53110	.42507	.34045	.27521	.64589	.64179	.54394	.53932	.46150	.45212	.32973	.38823
5.00	.90935 .58558	.58558	.50808	.45424	.39509	90269.	.69303	.62280	.61849	.57027	.56233	.50881	.50497
5.50	. 95534 . 60159	.60159	.54494	.51093	.46317	.71099	.70680	.65688	.65272	.62362	.61664	.57446	.57078
5.75	.96839 .60283	.60283	.55440	.52742	.48561	.71151	.70718	.66530	.66118	.63888	.63223	. 59607	. 59227
9.00	97740 . 60176	.60176	.56040	.53902	.50286	.70983	.70540	.67044	.66634	87679.	.64309	.61269	.60867
6.25	.98361	.59936	.56409	.54717	.51621	.70712	.70244	.67343	.66934	.65681	.65064	.62560	.62125
6.50	.98789 .59630	.59630	.56629	.55290	.52662	.70381	.69893	.67504	96029.	.66189	.65588	.63570	.63098
7.00	.99288	.58972	.56814	.55979	.54124	66969.	.69173	.67598	.67192	.66773	.66206	96679.	.64447
7.50	.99527	.58377	.56844	.56324	.55043	66069.	.68542	.67557	.67155	.67040	.66503	.65894	.65290
8.00	.99643	.99643 .57898	.56821	.56499	.55629	.68618	07089.	.67471	.67077	.67148	.66641	95799.	.65835
9.00	.99730	.57271	.56755	.56633	.56252	.67945	.67369	.67264	16899.	.67137	76999	.66977	.66426
10.00	. 99755 . 56952	.56952	.56711	99995.	.56515	.67486	79699.	.67032	.66701	18699.	00999.	.67056	.66618
20.00	. 99703 . 56655	.56655	.56653	.56653	.56655	.56655 .64309		.64067 .64242	.64024	.64241	.64020	.64304	86079.

 $^{\mathbf{a}}$ All quantities in a.u. Energies are negative and are relative to -32,00000.



Graphical Data. A-6.8. Xe_2 , Xe_2^* and Xe_2^+ potential energy curves including spin-orbit coupling.

Tabular Data. A-6.9. Selected Xe_2^+ and Xe_2^* vertical transition energies (eV).

		æ	cIp	CI-EPC
xe ²	$(1/2)_{\rm u} + (3/2)_{\rm g}$	1.03	0.99	0.96
	$+ 1(1/2)_g$	1.67	1.60	1.57
	+ II(1/2) _g	3.56	3.31	3.32
Xe2*d	0+ x0+ n	66.9		
	$l_u + x_0^+$	6.88		

a Reference 1.

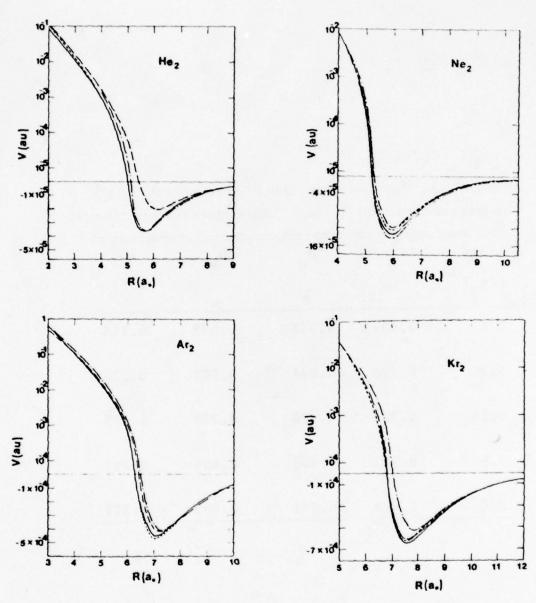
b Reference 2.

c Reference 3.

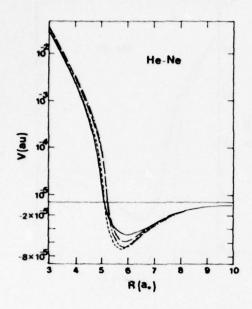
d A bound-free emission is observed at 7.3 eV.

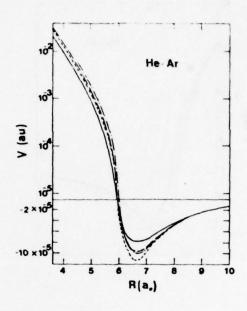
Tabular Data. A-6.10. Variation of the magnitude of the transition moment for Xe_2^* with internuclear distance (a.u.).

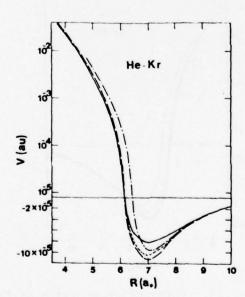
State R(a ₀)	1 _E ⁺ _u	¹ п	o _u +	1 _u
5.5	0.691	0.953	0.678	0.115
5.75	0.723	0.944	0.705	0.130
6.25	0.785	0.922	0.752	0.159
7.5	0.901	0.866	0.804	0.207
8.0	0.926	0.841	0.803	0.209



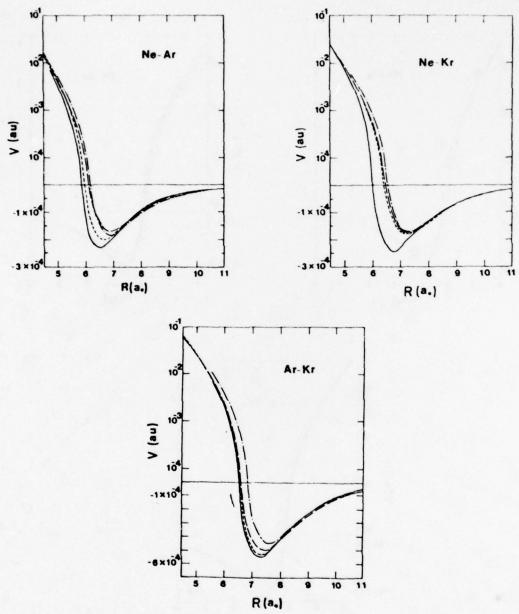
Graphical Data. A-6.11. Interaction energies for $^{1}\Sigma^{+}$ states of He₂, Ne₂, Ar₂, and Kr₂ as determined by experiment [solid line, Refs. (A-5.8) - (A-5.11)] and by various theoretical models [broken lines, Ref. (A-5.5)].







Graphical Data. A-6.12. Interaction energies of He-Ne $(^1\Sigma^+)$, He-Ar $(^1\Sigma^+)$ and He-Kr $(^1\Sigma^+)$ as determined by experiment [solid line, Ref. (A-5.12)] and by various theoretical models [broken line, Ref. (A-5.5)].



Graphical Data. A-6.13. Interaction energies of Ne-Ar $(^1\Sigma^+)$, Ne-Kr $(^1\Sigma^+)$, and Ar-Kr $(^1\Sigma^+)$ as determined by experiment [solid line, Refs. (A-5.13) and (A-5.14)] and by various theoretical models [broken lines, ref. (A-5.5)].

A-7. POTENTIAL ENERGY CURVES, ELECTRONIC ENERGIES, SPECTROSCOPIC CONSTANTS, AND ABSORPTION SPECTRA FOR Ne₂⁺, Ar₂⁺, Kr₂⁺, Xe₂⁺, AND ArKr⁺

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A-7. POTENTIAL ENERGY CURVES, ELECTRONIC ENERGIES, SPECTROSCOPIC CONSTANTS AND ABSORPTION SPECTRA FOR Ne₂⁺, Ar₂⁺, Kr₂⁺, Xe₂⁺ AND ArKr⁺.

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- C. F. Bender and N. W. Winter, "Theoretical Absorption Spectra of ArKr⁺," Appl. Phys. Letts. <u>33</u>, 29 (1978).

Tabular Data. A-7.1. Long-range-force interaction parameters for the noble gas dimer ions.

Species	a _o (bohr ³)	$\Sigma < r_i^2 > (bohr^2)$	<u>I (eV</u>)
Ne	2.66 a,b	9.699 ^d	21.564 e,f
Ne	(1.32) °	6.842	40.962
Ar	11.08	26.145	15.759
Ar	(6.52)	20.054	27.629
Kr	16.74	39.674	13.999
Kr ⁺	(10.78)	31.847	24.359
Xe	27.29	62.511	12.127
Xe ⁺	(18.90)	52.022	21.2

a R. R. Teachout and R. T. Pack, Atomic Data 3, 195 (1971).

$$\alpha_0 \sim \Sigma < r_i^2 > \frac{2}{r_i}$$

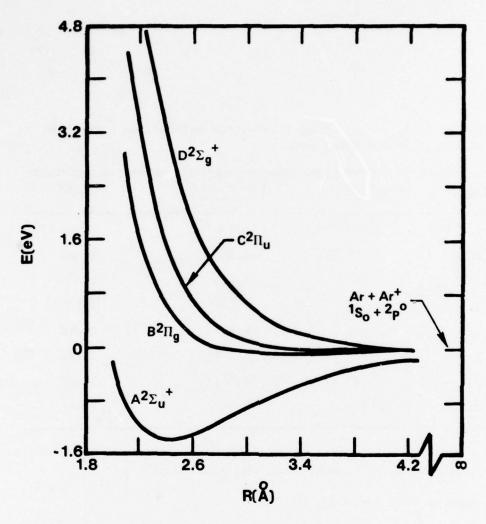
b A. Dalgarno, Adv. Physics <u>11</u>, 281 (1962).

The ion polarizabilities are scaled from the atomic $lpha_{0}$ using the hydrogenic form,

d Non-relativistic Hartree-Fock calculation.

e R. L. Kelly and D. E. Harrison, Jr., Atomic Data 3, 177 (1971).

f C. E. Moore, Nat. Bur. Std. (U.S.) Circ. 467 (1958).



Graphical Data. A-7.2. Ab initio potential energy curves for Ar_2^+ without inclusion of spin-orbit coupling.

Tabular Data. A-7.3. Potential energy curves for Ne $_2$ including spin-orbit coupling. Energies in eV relative to c.g. of Ne $_2^+$ at R = $^\circ$.

R (a.u.)	A 2 + Zu	m	B 21/28	2 2 1/2 B 2 1/2 C 13/2 C 2 1/2 D 2 + 1/2 D	C 21/2u	D 2+ 1/2u
2.8	-0.89497					
3.0	-1.28953	1.26194	1.32586	2.57256	2.63768	4.50598
3.2	-1.37990	0.48908	0.55283	1.43735	1.50265	3.06507
3.4	-1.31808	0.07755	0.14109	0.76574	0.83129	2.11391
3.6	-1.18232	-0.12882	-0.06558	0.37242	0.43830	1.47550
3.8	-1.01630	-0.21895	-0.15609	0.14705	0.21334	1.04125
0.4	-0.84617	-0.24597	-0.18362	0.02207	0.08890	0.74236
4.2	-0.68726	-0.24091	-0.17924	-0.04416	0.02338	0.53395
η·η	-0.54766	-0.22074	-0.15998	-0.07598	-0.00748	0.38739
9.4	-0.43046	-0.19535	-0.13579	-0.08868	-0.01897	0.28363
8	-0.03230	-0.03230 -0.03230	-0.03230	-0.03230	09790.0	09490.0

Tabular Data, A-7.4. Potential energy curves for ${\rm Ar}_2^+$ including spin-orbit coupling. Energies in eV relative to c.g. of ${\rm Ar}_2^+$ at ${\rm R}=^\infty$.

mergaco in contractor constituents	מים ביו	2 2				
R (a.u.)	A 2 + 1/2	B 2 13/2g	B 2 1/2R	c 2 13/2u	c 2 1/2u	D 25+ 1/2u
4.2	-1.18618	1.65365	1.76982	2.77055	2.89064	4.95560
4.4	-1.34226	ı	•	•	٠	•
7.6	-1.38227	0.44736	0.56260	1.14139	1.26240	2.81570
4.8	-1.34896	0.14654	0.26118	.0.69322	0.81483	2.14999
5.0	-1.27160	-0.03714	0.07676	0.39334	0.51563	1.65681
5.2	-1.16918	-0.14504	-0.03200	0.19416	0.31726	1.28605
5.4	-1.05453	-0.19620	-0.08425	0.07089	0.19489	1.01491
5.8	-0.82182	-0.22463	-0.11562	-0.05891	0.06740	0.64328
0.9	-0.71382	-0.21307	-0.10599	-0.08259	0.04512	0.52554
6.2	-0.61523	-0.19933	19160.0-	74960.0-	0.03290	0.43043
8	-0.05919	-0.05919	-0.05919	-0.05919	0.11837	0.11837

Tabular Data. A-7.5. Potential energy curves for ${\rm Kr}_2^+$ including spin-orbit coupling. Energies in eV relative to c.g. of ${\rm Kr}_2^+$ at R = $^{\omega}$.

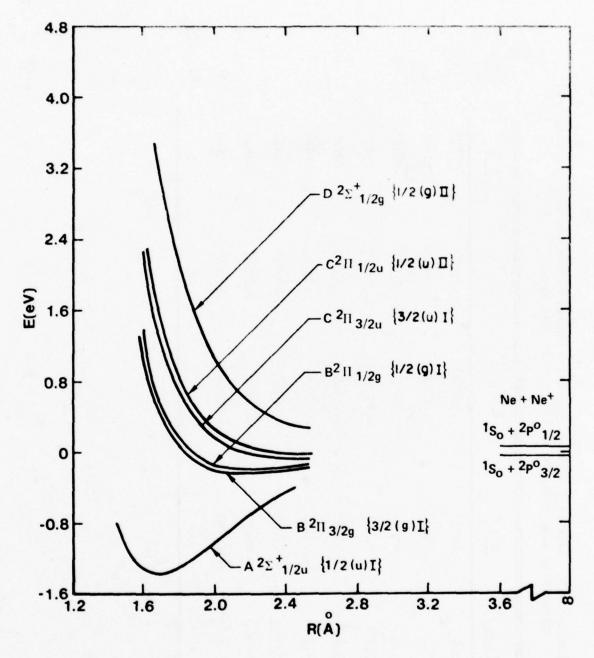
R (a.u.)	A 25+	В 2 13/29	B 2 1/28	C 2 113/21	C 2 1/2u	D 2 + 1/2m
4.8	-1.28087	1	1			1
5.0	-1.38709	0.69575	1.09151	1.43876	1.91284	3.18488
5.2	-1.41503	0.27628	0.66358	0.87603	1.35598	2.46023
5.4	-1.38910	0.00729	0.38423	0.48908	0.97546	1.92201
5.6	-1.32866	-0.16482	0.19960	0.22295	0.71627	1.51846
5.8	-1.24730	-0.28795	0.06150	0.02825	0.52948	1.19889
0.9	-1.15345	-0.33612	-0.00457	-0.08468	0.42439	0.98465
4.9	-0.95763	-0.39054	-0.10324	-0.22768	0.30020	0.58250
6.8	-0.77681	-0.38945	-0.15500	-0.28414	0.26501	0.52489
7.0	-0.69752	-0.37898	-0.17192	-0.27435	0.26591	0.18097
7.2	-0.62696	-0.36673	-0.18626	-0.29870	0.27285	0.45125
8	-0.22197	-0.22197	-0.22197	-0.22197	0.44393	0.44393

Tabular Data. A-7.6. Potential energy curves for Xe_2 including spin-orbit coupling. Energies in eV relative to c.g. of Xe_2^2 at $R=\infty$.

R (a.u.)	$A = \frac{2}{\Sigma} + \frac{1}{2}$	B 2 13/2g	B 2 1/28	c 2 13/2u	c 2 1/2u	D 2 1/2u
5.6	-1.40193		,	,		-
5.8	-1.48344	0.33100	0.95693	0.93646	1.92269	2.74968
0.9	-1.50867	0.02237	0.61482	0.52197	1.52369	2.25511
6.2	-1.49362	-0.16564	0.38771	0.24616	1.26243	1.89954
4.9	-1.45490	-0.33783	0.17473	0.00150	1.03543	1.59142
9.9	-1.39811	-0.44565	0.02261	-0.16640	0.88498	1.36717
6.8	-1.33076	-0.52015	-0.09755	-0.29043	0.77902	1.19677
7.0	-1.25/01	-0.55939	-0.18338	-0.37035	0.71648	1.07791
7.4	-1.10398	-0.58459	-0.29772	-0.45724	0.66367	0.93575
7.6	-1.03040	-0.58149	-0.33514	-0.47699	0.66026	0.89673
7.8	-0.95973	-0.57425	-0.36461	-0.48069	0.67123	0.87026
8.0	-0.89665	-0.56304	-0.38755	-0.49278	0.67575	0.85330
8.2	-0.83747	-0.54924	-0.40162	-0.49133	0.69129	0.84609
8	-0.43549	-0.43549	-0.43549	-0.43549	0.87098	0.87098

Tabular Data. A-7.7. Density functional potential energy curves for Ne $_2^+$ assuming Λ -S coupling. Energies in a.u. relative to E($^\infty$) = -256.3646 a.u.

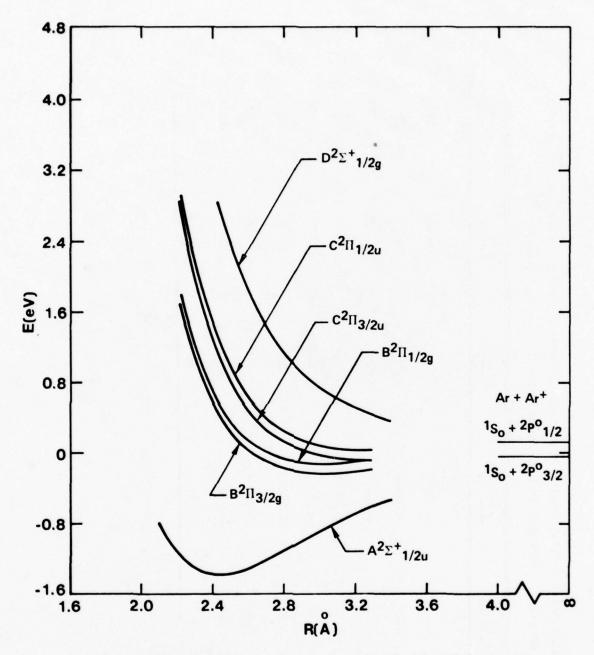
R (a.u.)	A ² E _u +	В ² П	0 2 n	D 2 E +
3.0	04737	9540.	.09573	.16557
3.2	05068	91610.	.05401	.11261
3.4	04840	10100.	.02933	.07765
3.6	0.640	00355	.01487	71450.
3.8	03729	-,00686	.00659	.03820
0.4	03101	00785	.00200	.02720
4.2	02515	-,00767	77000-	13610.
7.7	01998	-,00693	00161	01410.
4.6	01563	-,00599	00207	,01024
8	.0	.0	.0	0.



Graphical Data. A-7.8. Density functional potential energy curves for Ne_2^+ (spin-orbit effects included).

Tabular Data. A-7.9. Density functional potential energy curves for ${\rm Ar}_2$ assuming A-S coupling. Energies in a.u. relative to E ($^{\infty}$)² = -1053.0921.

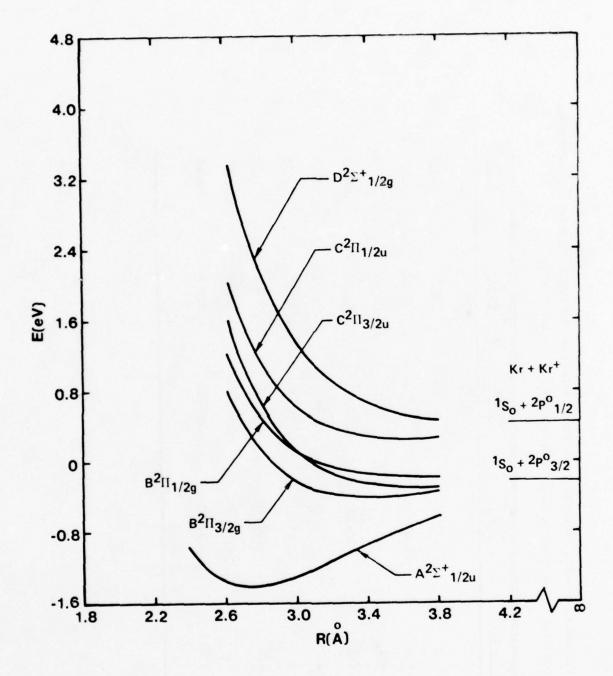
R (8.u.)	A ² E ⁺ u	В ² л	2 4 2 2 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	+ 3 D
4.2	04353	.06295	.10399	.18203
9.4	05070	.01862	.04412	.10336
4.8	04945	.00756	.02765	.07887
5.0	04659	.00081	.01663	.06072
5.2	04279	00316	.00931	.04707
5.4	03855	00504	.00478	.03706
5.8	02991	00608	.00001	.02330
0.9	02589	00566	00086	.01890
6.2	02221	00515	00137	.01532
8	0.	·	·	



Graphical Data. A-7.10. Density functional potential energy curves for Ar_2^+ (spin-orbit effects included).

Tabular Data. A-7-11. Density functional potential energy curves for Kr_2^+ assuming $\Lambda-S$ coupling. Energies in a.u. relative to $E(\infty)$ = -5503.6239.

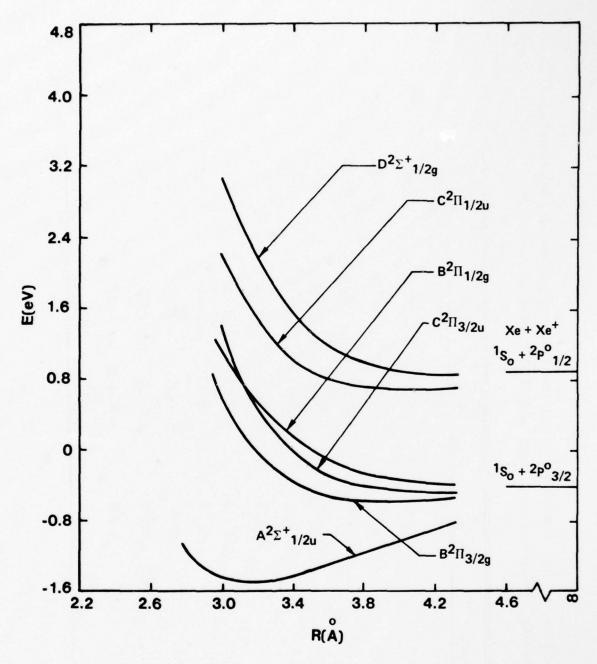
R (a.u.)	$\frac{A^2}{a}$	B 2 II	C 2n	D 2 +
5.0	04987	.03373	.06103	.11527
5.2	05068	.01831	.04035	.08833
5.4	04949	.00843	.02613	71890.
9.6	04701	.00210	.01635	.05288
5.8	04373	00243	.00920	65070.
6.0	03999	00420	.00505	.03206
4.9	03211	00620	00021	.01933
6.8	02468	00616	00229	.01159
7.0	02136	00577	00266	76800.
7.2	01835	00532	00282	06900
8	.0	.0	.0	·



Graphical Data. A-7.12. Density functional potential energy curves for Kr_2^+ (spin-orbit effects included).

Fabular Data. A-7.13. Density functional potential energy curves for Xe_2^+ assuming A-S coupling. Energies in a.u. relative to $E(\infty)$ = -14463.8615.

R(a.u.)	A 2 + 4	в 2п	2 2	+ 3 0
5.8	05028	.02817	.05042	70260.
0.9	05064	.01683	.03519	.07264
6.2	04955	26600.	.02505	.05613
.7.9	04748	.00359	90910.	.04531
9.9	04475	00037	68600.	.03541
6.8	04161	00311	.00533	.02750
7.0	03825	00455	.00239	.02142
7.4	03139	00548	00080	.01292
7.6	02808	00537	00153	00010.
7.8	02h9h	00510	00166	.00768
0.0	02202	00469	00211	.00580
8.2	01932	00418	00205	.00451
8	.0	.0	.0	



Graphical Data. A-7.14. Density functional potential energy curves for Xe_2^+ (spin-orbit effects included).

Tabular Data. A-7.15. Spectroscopic constants for Ne_2^+

State	T _e (eV)	we (cm-1)	T_e (eV) ω_e (cm ⁻¹) $\omega_e X_e$ (cm ⁻¹)	$\alpha_e(cm^{-1})$ $r_e(A)$	r _e (A)	$B_{e}(cm^{-1})$ $D_{e}(eV)$ $D_{o}(eV)$	D _e (eV)	D _o (eV)
D^{2} Σ^{+}	544.4	(vertical	vertical excitation energy, repulsive curve)	ergy, repuls	ive curve			
c 2 1/20	1.359	122.5	4.8	9910.0	2.50	0.2665	0.085	0.078
c 2113/2u	1.287	103.9	8.7	0.0194	2.54	0.2579	090.0	0.054
B 21/2g	1.195	5.945	0.6	0.0125	2.15	0.3626	0.152	0.137
в 2п3/28	1.132	250.8	9.6	0.0122	2.14	0.3634	0.215	0,199
A 25+	0.0	0.765	6.1	0600.0	1.69	0.5840	1.347	1.310

Tabular Data. A-7.16. Spectroscopic constants for Ar_2^+ .

State	T _e (eV)	$T_e(eV) = \omega_e(cm^{-1}) = \omega_e$	$\omega_{\rm e} \chi_{\rm e} ({\rm cm}^{-1}) \alpha_{\rm e} ({\rm cm}^{-1}) r_{\rm e} (A) B_{\rm e} ({\rm cm}^{-1}) D_{\rm e} ({\rm eV}) D_{\rm o} ({\rm eV})$	$a_e^{(cm^{-1})}$	r _e (A)	$B_{e}(cm^{-1})$	D _e (eV)	D _o (eV)
D 2,+ 1/2g	4.198		(vertical excitation energy, repulsive curve	n energy,	repulsi	re curve)		
c 2 1/2u	1.413	62.4	6.3	7400.0	3.40	0.0732	0.087	0.084
c 2 3/2u	1.285	53.7	3.7	0.0043	3.40	0.0732	0.037	0.034
B 2 1/2g	1.264	146.9	12.0	0.0030	3.02	0.0924	0.058	0.049
B 213/28	1.155	153.7	10.1	0.0024	3.02	0.0927	0.167	0.158
A 2r+	0.0	297.9	1.7	0.0011	2.43	0.1428	1.322	1.304

Tabular Data. A-7.17. Spectroscopic constants for Kr_2 .

State Te	(eV)	w (cm ⁻¹)	$\omega_{e^{X}e^{(cm^{-1})}}$	a (cm 1)	re(A)	$B_{e}(cm^{-1})$ $D_{e}(eV)$ $D_{o}(eV)$	D _e (eV)	D (eV
2+ 2 1/28	3.875	(vertical	(vertical excitation energy repulsive curve	nergy repuls	ive curve			
B2n1/2g	2.079	(vertical	(vertical excitation energy, repulsive curve	nergy, repul	sive curv	e)		
c 211/2u	1.679	70.2	1.3	0.0004	3.64	0.0304	0.179	0.175
c 2 3/2u	1.115	51.7	7.0	0.0001	3.85	0.0271	110.0	0.074
B 713/28	1.019	78.0	1.9	700000	3.48	0.0333	0.173	0.168
A 2 + 0.0	0.0	176.7	0.7	0.0002	2.75	0.0533	1.192	1.181

Tabular Data. A-7.18. Spectroscopic constants for Xe_2 .

State	Te(eV)	E (Cm-1)	w X (cm ⁻¹)	$\alpha_e^{(cm^{-1})}$	r _e (A)	$B_e(cm^{-1})$ $D_e(eV)$ $D_o(eV)$	D (eV)	Do(eV)
D 2 + 3.764	3.764	(vertical	(vertical excitation energy, repulsive curve)	energy, rej	pulsive cur	.ve)		
c 21/2u	2.169	54.5	0.3	0.0002	3.97	0.0163	0.209	0.206
в 2 1/28	2.123	(vertical	(vertical excitation energy, repulsive curve)	energy, rei	pulsive cur	ve)		
c 2 13/2u 1	1.034	58.5	0.3	0,000	7.00	0.0160	0.042	0.038
в ² п _{3/2g} о.	0.923	49.7	0.3	0.0003	3.91	0.0168	0.149	0.146
A 2 1/2u 0.0	0.0	117.2	7.0	0.0001	3.18	0.0253	1.072	1.065

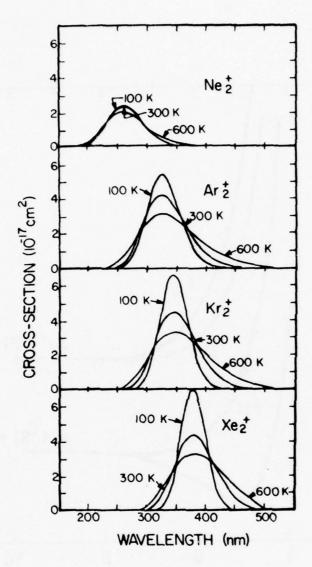
Tabular Data. A-7.19. Summary of spectroscopic constants for the A $^2\Sigma^+$ state of the noble gas dimer ions.

Ion	$\frac{D_{e}(eV)}{e}$	(-so) D _e (ev)	< <u>r >(a.u.)</u>	{-S0}* R (a.u.)
Ne ₂ +	1.35	1.37	0.965	3.19
Ar 2	1.32	1.40	1.663	4.59
Kr ₂ +	1.19	1.39	1.952	5.17
Xe ₂ +	1.07	1.38	2,338	5.94

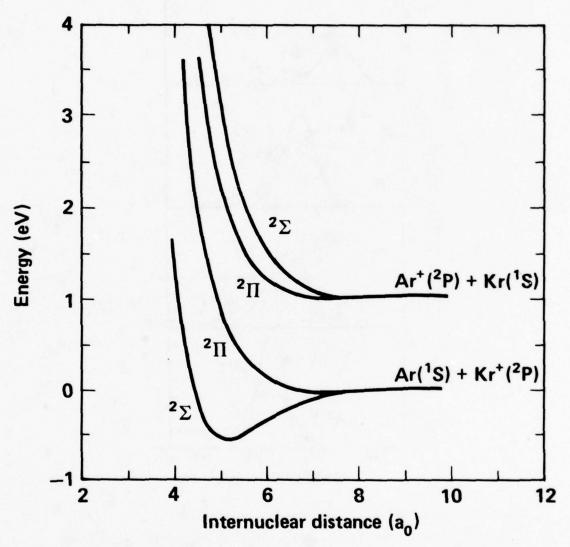
*{-50}: Without spin-orbit effects.

Tabular Data. A-7.20. Absorption cross sections (in 10^{-18} cm²) for the I(1/2) $_{\rm u}$ + II(1/2) $_{\rm g}$ transition in Ne₂, Ar₂, Kr₂, and Xe₂ based on <u>ab initio</u> calculated spectra shifted to The unshifted cross sections for Art, Kr2, coincide with experimental absorption maxima. and Xe_2^+ are shown in parentheses.

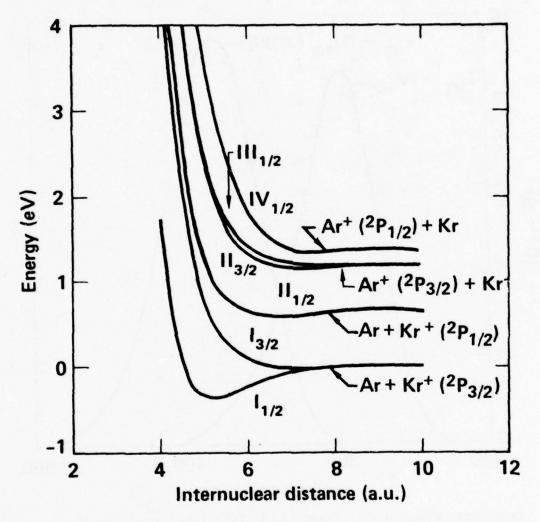
		KrF 248 nm	XeBr 282 nm	XeCl	XeF 352 nm
	(300 °K)	23	17	7.4	0.96
	(%.009)	21	15	8.6	2.5
Art	(300°K)	10 (1.2)	44 (18)	39 (38)	8.7 (31)
	(Y. 009)	14 (3.4)	34 (19)	32 (30)	15 (27)
	(300°K)	0.31 (0.061)	14 (5.1)	40 (24)	36 (42)
,	(800°K)	1.7 (0.45)	19 (9.4)	32 (23)	31 (31)
Xe;	(300°K)	$0.0031 (7.4 \times 10^{-8})$	1.7 (0.041)	16 (2.9)	48 (31)
	(H° 009)	$0.041 (1.8 \times 10^{-7})$	5.9 (0.14)	18 (7.0)	34 (27)



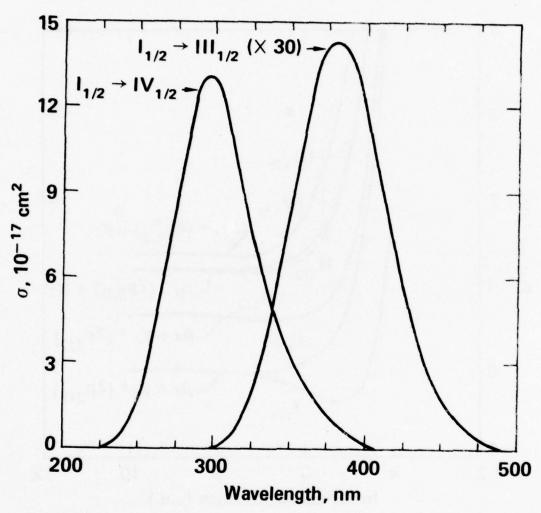
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A-8. POTENTIAL ENERGY CURVES, VIBRATIONAL LEVELS, TRANSITION MOMENTS, FLUORESCENCE AND EINSTEIN TRANSITION PROBABILITIES FOR NeF, ArF, ArCl, KrF, and KrCl. WAVENUMBERS, FRANCK-CONDON FACTORS, AND Rⁿ - CENTROIDS FOR XeF

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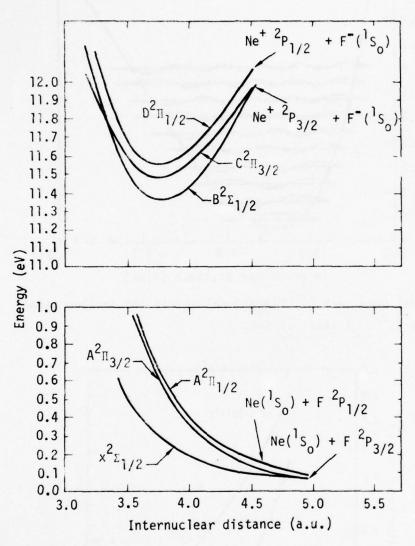
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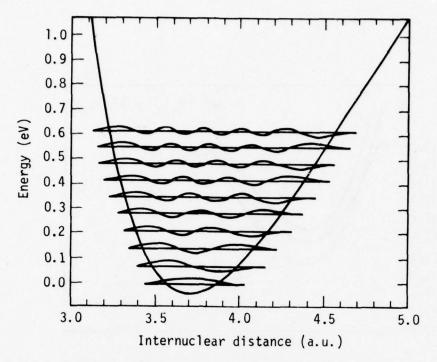
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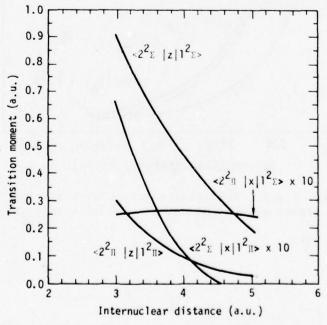
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- J. R. Murray and H. T. Powell, "KrCl Laser Oscillation at 222 nm," Appl. Phys. Letts. <u>27</u>, 252 (1976).



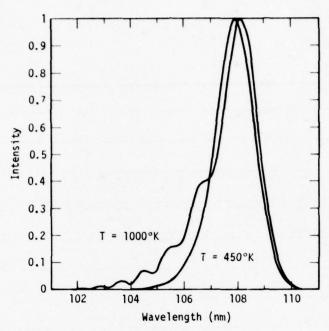
Graphical Data. A-8.1. Potential energy curves for the covalent and ion-pair states of NeF including spin-orbit coupling.



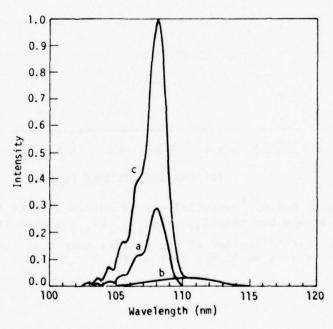
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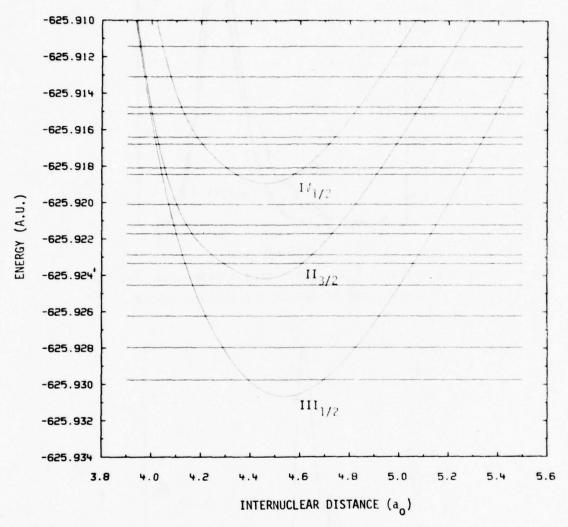
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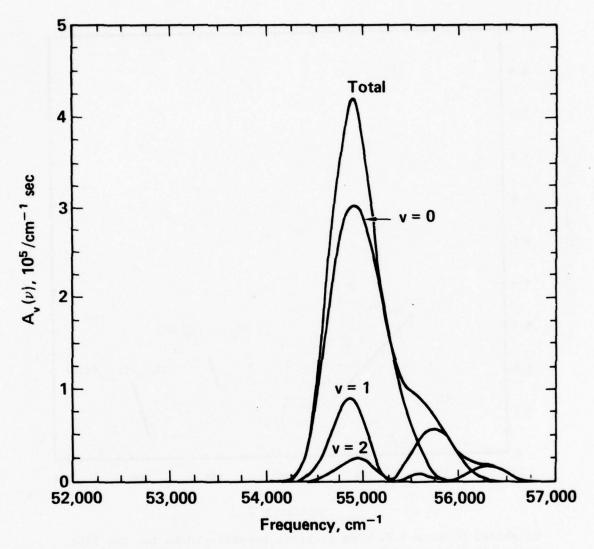
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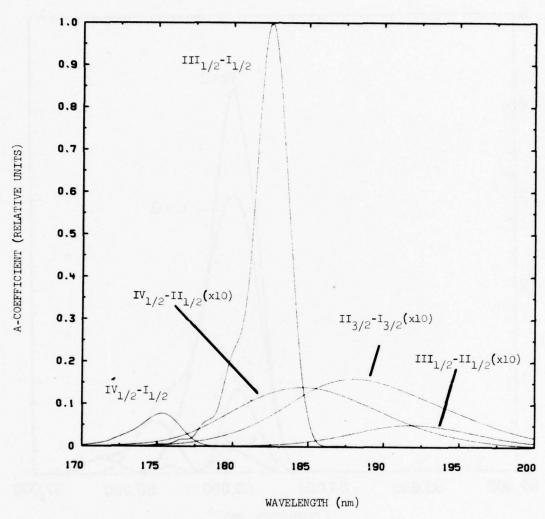
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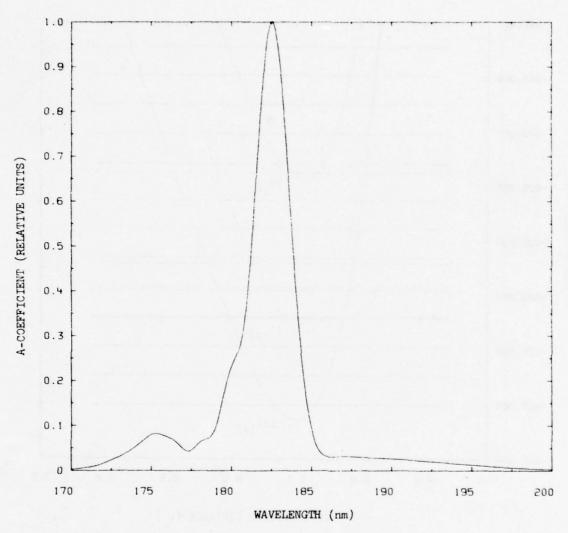
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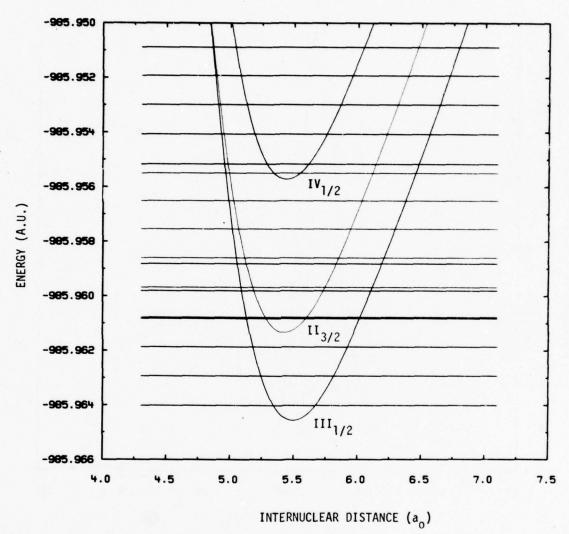
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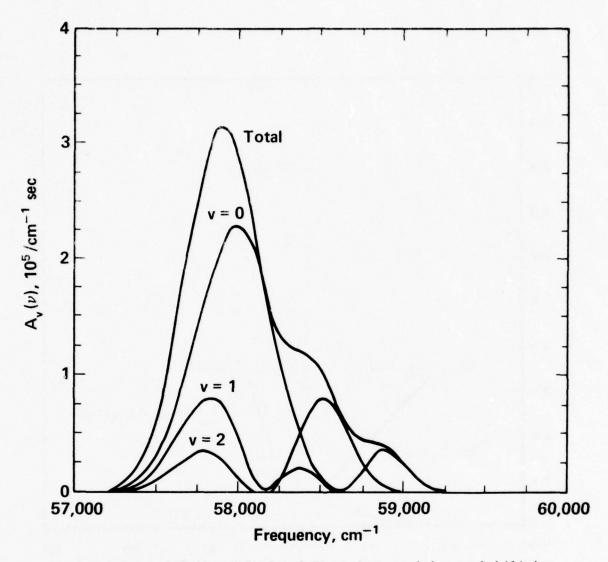
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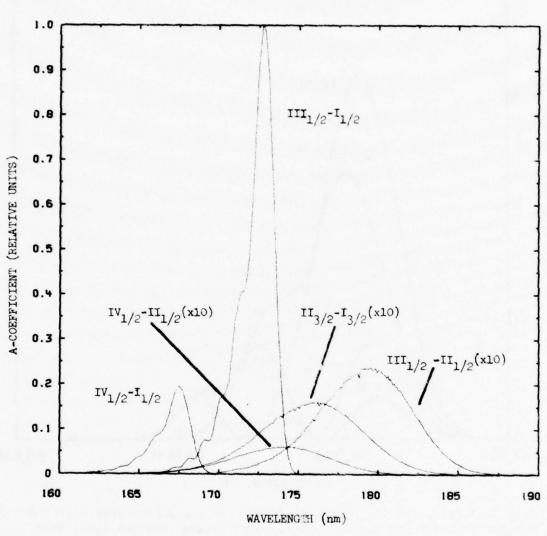
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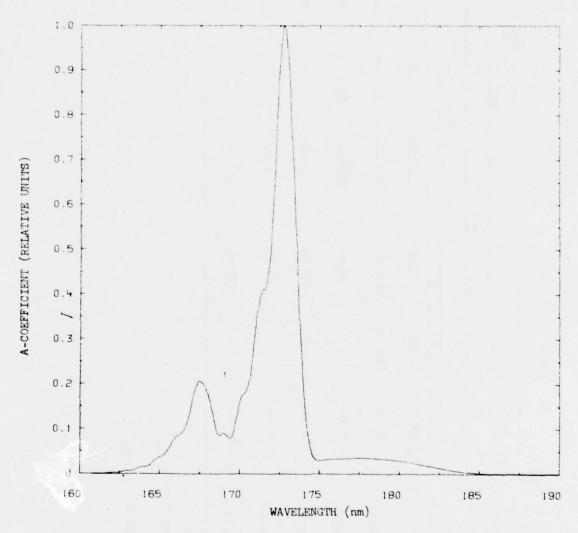
Graphical Data. A-8.10. The potential energy curves and six lowest vibrational levels for the $\rm II_{3/2}$, $\rm III_{1/2}$, and $\rm IV_{1/2}$ states of ArCl. To facilitate identification of the levels note that level separation is almost equal for each state.



Graphical Data. A-8.11. Calculated Einstein transition probabilities (A-coefficients) for the $III_{1/2}$ - $I_{1/2}$ transition from the first four vibrational levels of the $III_{1/2}$ state of ArCl. Each curve has been weighted by a Boltzmann factor for T = 450°K.



Graphical Data. A-8.12. The Einstein A-coefficients for the five strongest bands of ArCl.



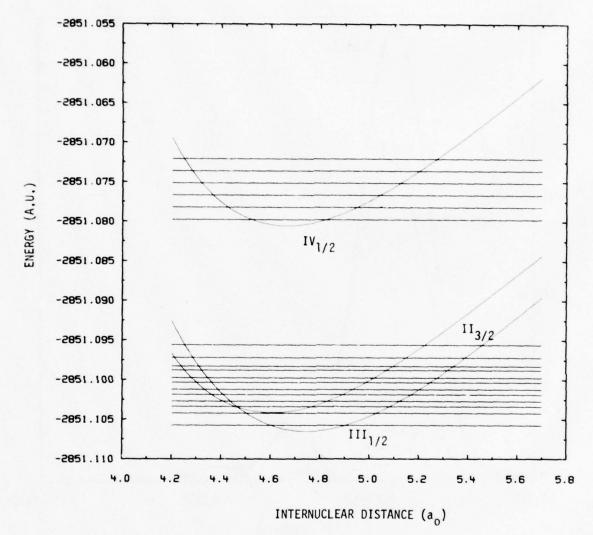
Graphical Data. A-8.13. The total Einstein A-coefficient for ArCl obtained by summing the contributions from the five strongest transitions with equal weightings.

Tabular Data. A-8.14. Comparison of ArF and ArCl emission features.

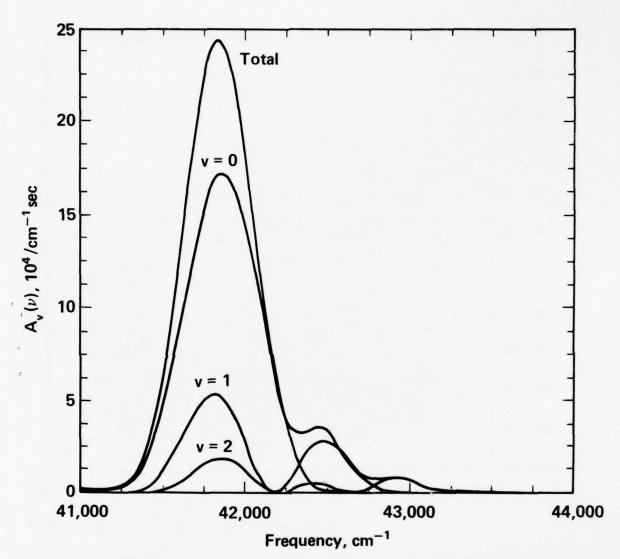
Transition		ArF			Arc1**	
	λ calc.	γ exp.	T calc.	λ calc.	γ exp.	T calc.
$B^2\Sigma_{1/2} + X^2\Sigma_{1/2}$	183 nm	пп 190	3.6 ns	173 nm	174 nm	4.4 ns
$D^2\Pi_{1/2} + X^2\Sigma_{1/2}$	175 nm		34 ns	167 nm	169 nm	su 61
$c^{2}\pi_{3/2} + A^{2}\pi_{3/2}$	188 nm		53 ns	175 nm		su 62
$D^2 \pi_{1/2} + A^2 \pi_{1/2}$	185 nm		94 ns	174 nm		223 ns
$B^2\Sigma_{1/2} + A^2\Pi_{1/2}$	194 nm		227 ns	180 nm		62 ns

* Evaluated at $R = 4.5 a_0$

** Evaluated at $R = 5.5 a_0$

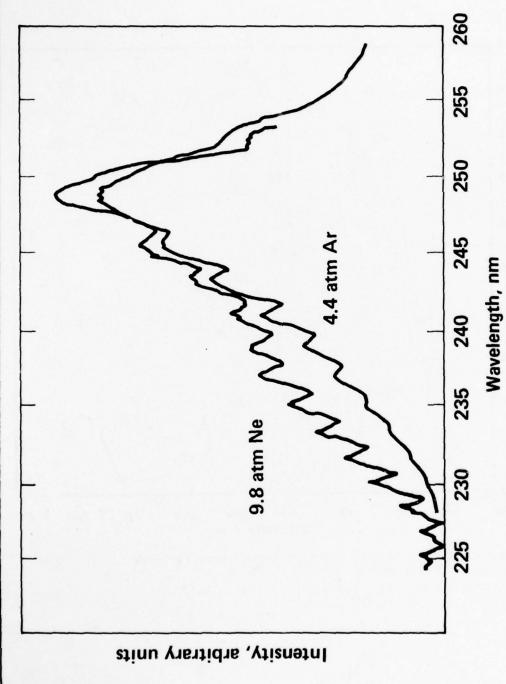


Graphical Data. A-8.15. The potential energy curves and six lowest vibrational levels for the ${\rm II}_{3/2}$, ${\rm III}_{1/2}$, and ${\rm IV}_{1/2}$ states of KrF including the positions of the vibrational levels for each state. To facilitate identification of the levels, note that level separation is almost constant for each state.

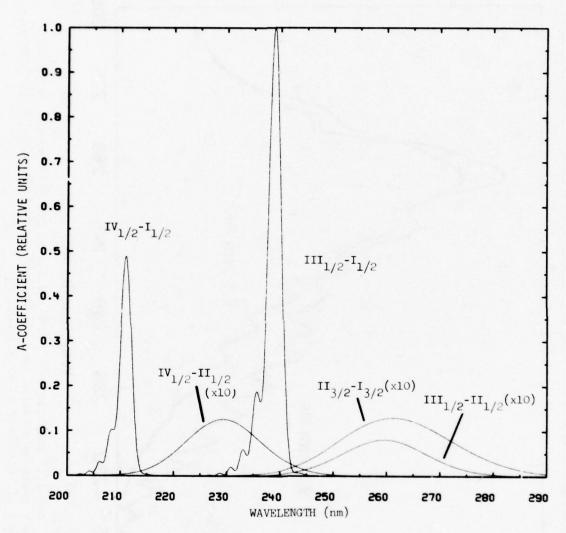


Graphical Data. A-8.16. Calculated Einstein transition probabilities (A-coefficients) for the $III_{1/2}$ – $I_{1/2}$ transition from the first four vibrational levels of the $III_{1/2}$ state of KrF. Each curve has been weighted by a Boltzmann factor for T = 450°K.

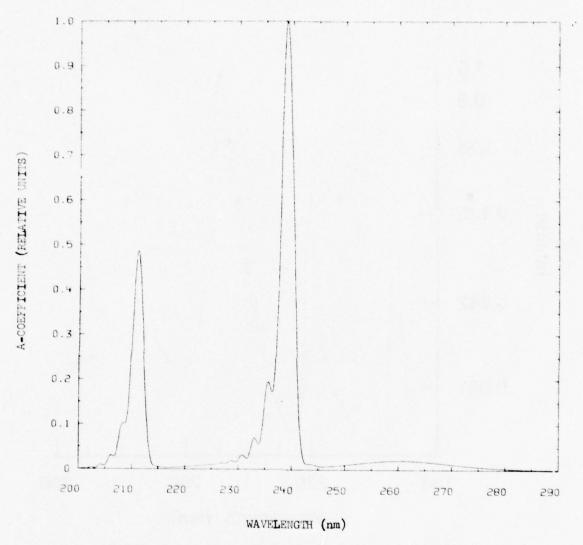
COMPARISON OF THE KrF III 1/2 + 1 1/2 TRANSITION WITH Ne AND Ar AS BUFFER GASES



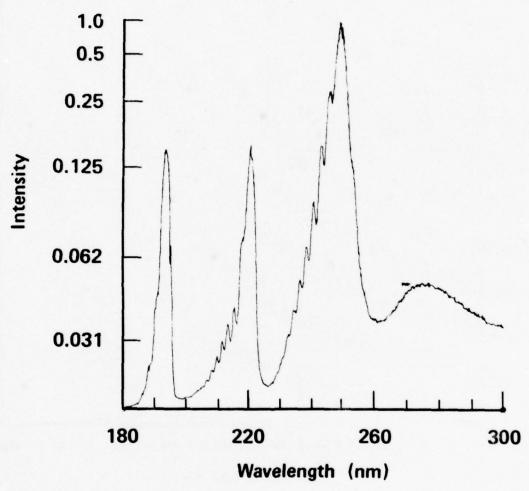
and Ar as diluent gases as measured by J. R. Murray and H. T. Powell (in Electronic Graphical Data, A-8.17. Comparison of the experimental KrF fluorescence using Ne Transition Lasers II, edited by L. E. Wilson).



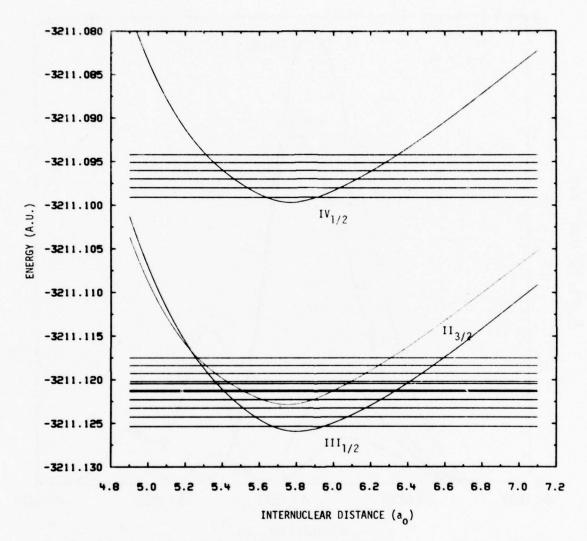
Graphical Data. A-8.18. The Einstein A-coefficients for the five strongest bands of KrF.



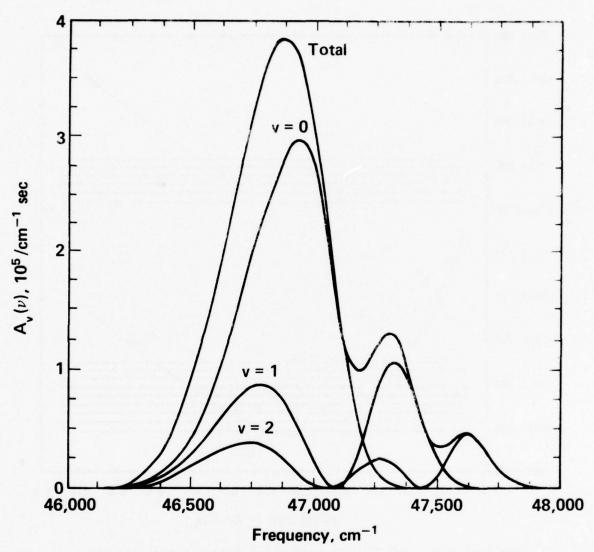
Graphical Data. A-8.19. The total Einstein A-coefficient for KrF obtained by summing the contributions from the five strongest transitions with equal weighting.



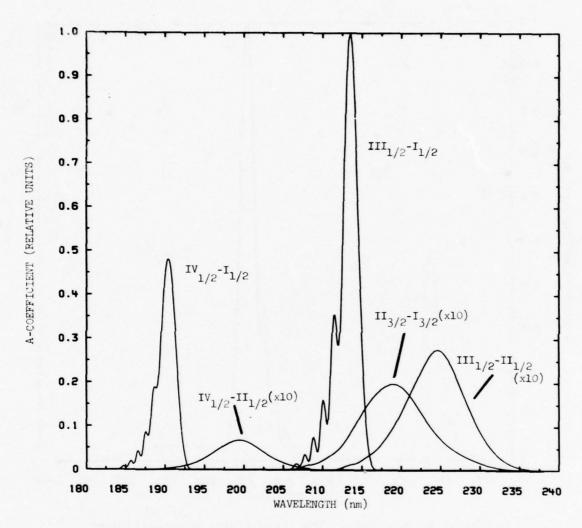
Graphical Data. A-8.20. KrF fluorescence spectrum.



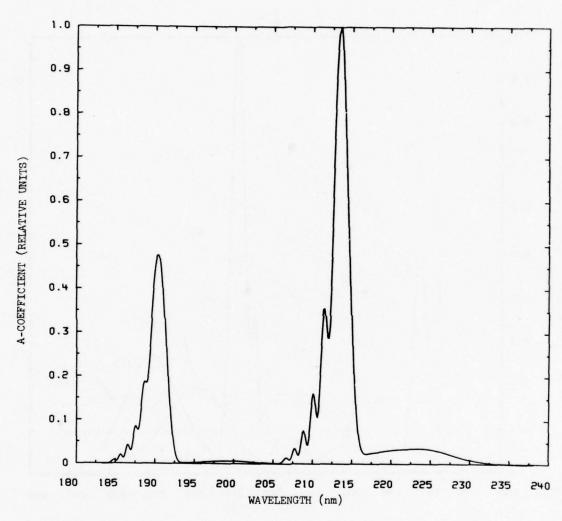
Graphical Data. A-8.21. The potential energy curves and six lowest vibrational levels for the ${\rm II}_{3/2}$, ${\rm III}_{1/2}$, and ${\rm IV}_{1/2}$ states of KrCl. To facilitate identification of levels, note the level separation is almost constant for each state.



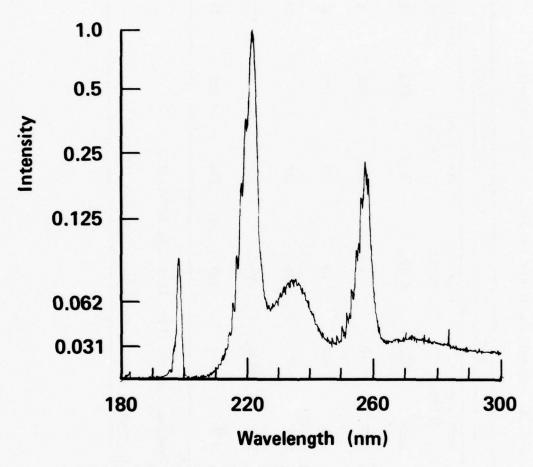
Graphical Data. A-8.22. The Einstein A-coefficient for the III $_{1/2}$ - $_{1/2}$ transition for KrCl in absolute units. Each curve has been weighted by a Boltzmann factor for T = 450°K.



Graphical Data. A-8.23. The Einstein A-coefficients for the five strongest bands of KrCl.



Graphical Data. A-8.24. The total Einstein A-coefficient for KrCl obtained by summing the contributions from the five strongest transitions with equal weightings.



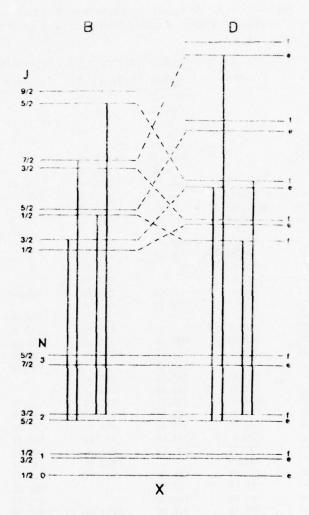
Graphical Data. A-8.25. KrCl fluorescence spectrum.

Tabular Data. A-8.26. Comparison of KrF and KrCl emission features.

		KrF			KrC1	
Transition	Wavelength (nm)	ч	Lifetime (nsec)	Wavelength (nm)		Lifetime (nsec)
	Calc ^a	Exp	Calca	Calc	Exp	Calc
$B^2\Sigma_{1/2} + X^2\Sigma_{1/2}$	239	248	7	214	222	7.9
$D^2 \pi_{1/2} + x^2 \Sigma_{1/2}$	211	220	13	191	199	11
$c^2 \pi_{3/2} + A^2 \pi_{3/2}$	264	~275	75	220		87
$D^2 \pi_{1/2} + A^2 \pi_{1/2}$	228	~236	96	200		278
$B^2\Sigma_{1/2} + A^2\Pi_{1/2}$	259		180	226	235	7.1

 $^{\rm a}{\rm P}$. J. Hay and T. H. Dunning, Applied Phys. Lett. 28, 649 (1976).

bj. R. Murray and H. T. Powell, Applied Phys. Lett. 29, 252 (1976).



Graphical Data. A-8.27. Abbreviated rotational level diagram for X, B, and D states of XeF, illustrating theoretically predicted branch structures for B-X and D-X transitions. The energies are arbitrary, with X levels taken as K'' with α = -0.135, and B and D levels taken as K'e'f with δ_B = 1.87 and δ_D = -0.87. In our notation the illustrated transitions for each system are, from left to right, $P_e(2)$, $R_e(2)$, $P_f(2)$, and $R_f(2)$.

Tabular Data. A-8.28. Wavenumbers (cm $^{-1}$) of assigned lines in 1-2 band of XeF B \rightarrow X transition.

N'	P_f branch	P, branch	R, branch	R, branch
4		28770.77		
5		770.02		
6				28 772.78
7	28769.85			
9		766,63		
10		765.61	28774.05	
11		764.54	773.73	
12		763.41	773.44	770.43
13	765.00	762.23		769.85
14	763.97	760.99	772.59	
15	762.87	759.68		
16		758.31		
17	760.56	756.88		
18	759.32	755.38	770.31	
19	758.01		769.55	
20	756.65		768.75	
21	755.25	750.62	767.89	762.87
22		748.93	766.96	
23				760.56
24	750.62		765.00	759.32
25	748.93	743.52	763.97	758.01
26		741.57	762.87	756.65
27		739.61		755,25
28	743.64	737.55	760.43	
29	741.80	735.46	759.16	
30	739.89	733.34	757.81	750.75
31	737.95	731.14	756.43	749.18
32	735.92	728.91	754.99	747.52
33	733.86	726.66	753.49	745.81
34	731.74	724.28	751.96	744.06
35	729.57		750.38	742,27
36	727.37	719.50	748.74	740.43
37	725.12	717.05		738.55
38	722.80	714.50		736.62
39	720.44	711.95	743,64	734.65
40	718.05	709.34	741.80	732,64
41	715.65	706.71	739.89	730.58
42	713.13	704.07		728.50
43	710.64	701.31	736.06	726,36
44	708.09	698.58	734.09	724.28
45	705.51	695.80	732,09	
46	702.84	693.02	730.03	719.86
47		690.23	727.99	717.63
48	697.48	687.33	725.83	715,41
49	694.75	001.00	723.69	713.13
50	692.02		721.51	710.91
51	000.00		719,32	120.31
52			717.05	
53			714.81	

Tabular Data. A-8.29. Franck-Condon factors $(\times 10^3)$ for B-X system of XeF. Successive entries for each band are values for N' = N" = 0, 20, 30, 40, 50, 60, 70.

υ"	v'=0	1	2	3	4	5
0	3	8	15	24	32	41
	4	9	17	25	34	43
	4	10	19	28	36	4
	5	12	21	31	40	41
	7	15	25	35	45	52
	10	20	32	42	51	51
	16	27	40	51	59	64
1	60	85	101	99	86	6
	66	90	104	99	85	6
	75	96	108	100	83	6
	90	105	113	100	80	5
	114	116	118	97	74	5
	151	127	121	91	64	3
	211	133	121	78	50	2
2	323	129	68	16	1	
	345	122	62	12	0	
	372	110	53	7	0	1
	412	91	42	2	1	13
	463	63	28	0	5	20
	521	27	14	4	12	3
	567	0	5	24	20	4:
3	489	20	12	68	40	3
	480	37	14	74	37	2
	463	65	15	81 ′	31	2
	427	119	15	89	22	1
	360	214	10	97	9	1:
	249	354	1	104	0	
	98	479	1	109	22	•
4	77	518	11	24	43	
	53	526	25	22	59	
	29	517	50	20	80	
	6	468	103	20	116	
	1	343	184	23	165	
	30	129	256	29	206	2
5	34	31	401	39	123	7
	39	8	373	52	117	9
	42	0	312	68	105	13
	38	29	193	80	80	173
	19	101	41	64	34	170
6	0	116	26	103	15	12
	1	97	66	59	8	8
	4	62	120	18	2	43
	10	13	154	1	2	,
7	4	37	30	124	4	38
	1	47	4	112	8	50
	0	45	4	73	10	47
8	3	5	57	41	4	
	2	14	22	57	0	
9	2	0	44	8	12	,

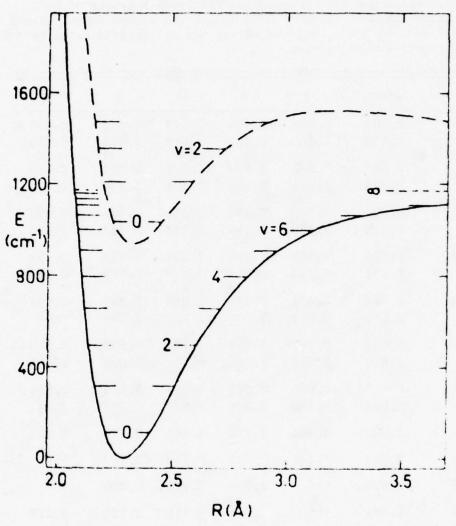
 $a_{(v'',N'')}$ levels (7,30), (6,40), (5,50), (4,50), (4,60), (3,60), (3,70), (2,70), and (1,70) lie above the dissociation limit; hence they can rotationally predissociate.

Tabular Data. A-8.30. Franck-Condon factors (\times 10³) for D-X system of XeF. Multiple entries, where they occur, are for N' = N" = 0, 20, and 30, successively.

e **	t. , = 0	1	2	3	4	5
0	75	96	111	111	104	9:
	81	100	114	112	105	92
	6.9	105	117	114	105	9
1	425	114	54	8	0	
	443	106	49	6	0	
	464	94	43	3	1	
2	441	105	27	88	35	23
	425	130	26	91	31	2:
	401	165	25	93	26	15
3	16	535	68	7	85	14
	9	516	92	7	98	11
	2	482	126	7	114	
4	34	0	401	85	81	122
	34	5	356	101	78	144
	32	20	291	118	73	171
5	2	76	89	100	33	100
	4	59	125	61	27	76
	6	37	166	25	18	46
6	1	42	8	182	4	18
	0	44	0	167	11	2€
	0	41	8	126	20	34
7	2	9	46	66	17	2
	1	14	22	86	3	(
	0	18	4	86	0	2
8	1	1	40	11	36	5
	1	4	24	28	13	2
9	1	0	26	1	33	3
0	0	0	16	0	24	1

Tabular Data, A-8.31. R centroids (A) for B-X system of XeF. The first entry is for N' = N'' = 0, and the second (where given) is for N' = N'' = 40. Omitted values are ill defined owing to weak Franck-Condon overlap.

v"	v'=0	1	2	3	4	5
0	2.536	2.494	2.466	2.443	2,423	2,406
	2.546	2.500	2.472	2.448	2.428	2.410
1	2.565	2.508	2.479	2,453	2.432	2,413
	2.576	2.511	2.485	2.456	2,436	2,416
2	2.600	2.499	2.496	2.435	2.404	2.458
	2.613	2.476	2.515	2.344	2,443	2.450
3	2.650	2.858	2.326	2.536	2.412	2.458
	2.673	2.730	2.198	2.572	2,329	2.514
4	2.785	2,683	3.352	2.884	2.702	2.091
	3,131	2,698	2,877	3.162	2.712	•••
5	2,592	2,877	2.714	3.182	2.839	2.899
	2,698	2,518	2.698	2.941	2.985	2.828
6	•••	2,695	2.640	2.665	3,361	2.856
	2,588	2,880	2.699	•••	2,657	3,444
7	2,830	2,604	2.775	2.742	3.779	2.708
8	2.724	2.445	2.725	2.758	2,257	•••
9	2.674	•••	2.704	2.771	2,622	•••
10	2.641		2.689	2.811	2.700	3.617



Graphical Data. A-8.32. Potential curves and vibrational energy levels for X state of XeF: rotationless potential (solid) and effective potential for N=70.

Tabular Data. A-8.33. Spectroscopic parameters (cm $^{-1}$) for X, B, and D states of XeF. Standard errors (lo, in parentheses) from the vibrational parameter determination are given in terms of last significant digits.

	X	В	ν
T.	0	25 811.0(7)	38 051,4(7)
Cu1(2,)	225, 40(150)	309,02(11)	350,14(19)
cuz(- wexe)	-10.874(1000)	-1.505(9)	-1.899(18)
Cus	0.2981(2700)		
CW	- 0, 08125(3100)		
Cus	0.004963(1330)		
D _e	1175(20)	42 783(20)	44 080(20)*
$C_{r1}(B_{e})$	0.19326b	0.14670	0.1608
cr2(-a,)	-6.985×10^{-3}	- 9.9×10 ⁻⁴	-1.20×10 ⁻³
C+3	1.596×10 ⁻⁴		
C+4	-7.167×10^{-5}		
R _e (Å)	2.293	2,631	2,513
$c_{a1}(D_e)$	5.36×10-7	1.32×10^{-7}	1.36×10 ⁻⁷
ca	1.53×10 ⁻⁷	1.6×10^{-10}	1.4×10 ⁻¹⁰
ca	-3.45×10^{-8}		
CH	1.08×10 ⁻⁸		
CA1(H)	-5.6×10^{-12}	-4.4×10^{-14}	-8.1×10^{-14}
CA2	-1.48×10^{-11}		
CAS	6.6×10 ⁻¹²		
C _{M4}	-1.9×10^{-12}		
۵	- 0.04°		
8		1.82	- 0.82d

^aDissociation to F⁻(1 S) + Xe⁺(2 P $_{3/2}$) for B state, Xe⁺(2 P $_{1/2}$) for D state.

^bRotational and centrifugal distortion parameters for X state valid for v'' = 0-6.

^cFrom analysis of 1-2 band only.

^dCalculated from δ_B , using $\delta_B + \delta_D = 1$.

Tabular Data. A-8.34. Spectroscopic constants (cm $^{-1}$) for 1-2 band of XeF B-X system, from least-squares fit of assigned lines having N \leq 40. Standard errors (1 σ , in parentheses) are in terms of last significant digits.

28 773. 070(7)
0.14521(4)
$(1.35 \times 10^{-7})^{2}$
1.820(17)
0.17568(5)
$9.67(12) \times 10^{-7}$
$(-3.0 \times 10^{-11})^a$
-0.041(14)
$-4.3(11) \times 10^{-10}$
0.023

 $^{^{\}mathrm{a}}$ Calculated at the outset and held fixed in the fit.

A-9. POTENTIAL ENERGY CURVES, ELECTRONIC ENERGIES, SPECTROSCOPIC CONSTANTS, AND TRANSITION MOMENTS FOR ${\rm Ar}_2{\rm F}$ and ${\rm Kr}_2{\rm F}$

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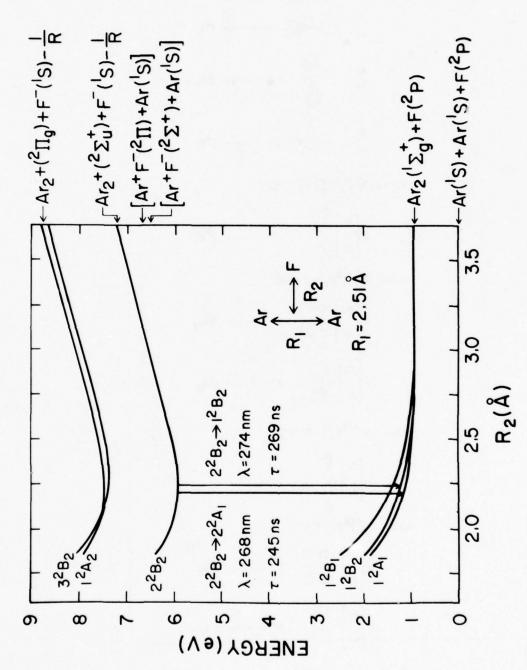
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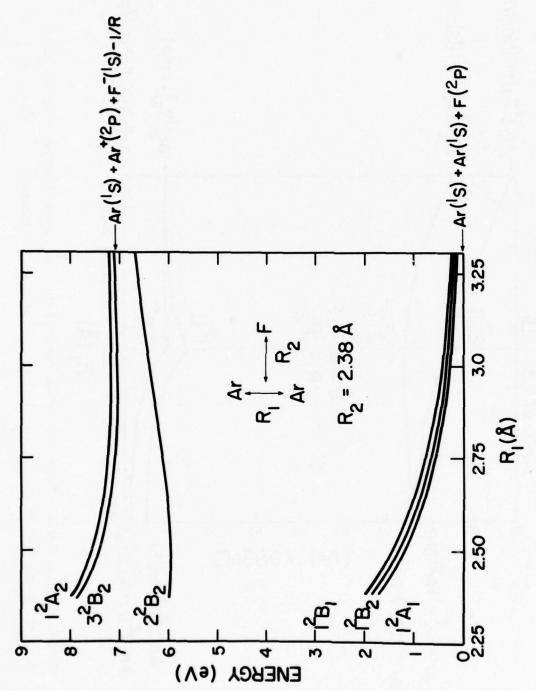
A-9. References:

1. W. R. Wadt and P. J. Hay, "Electronic States of Ar_2F and Kr_2F ," J. Chem. Phys. <u>68</u>, 3850 (1978).

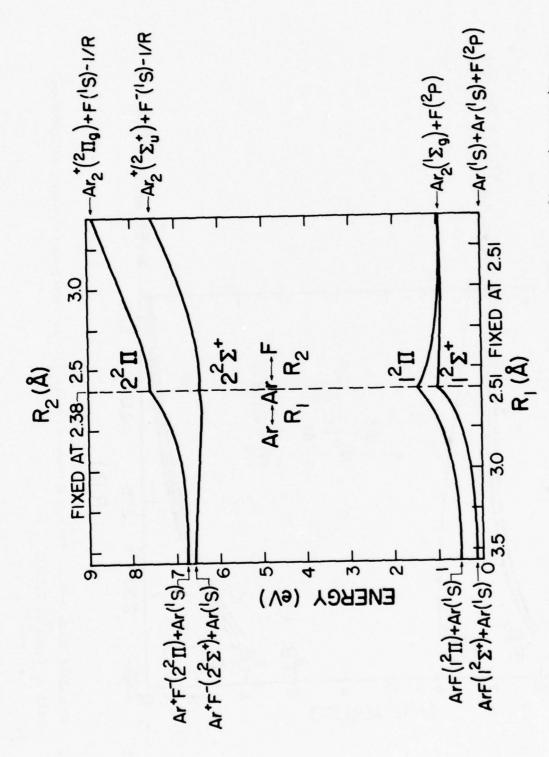
Graphical Data. A-9.1. Schematic orbit representation of the nine lowest electronic states of Ar₂F for isosceles triangle geometries.



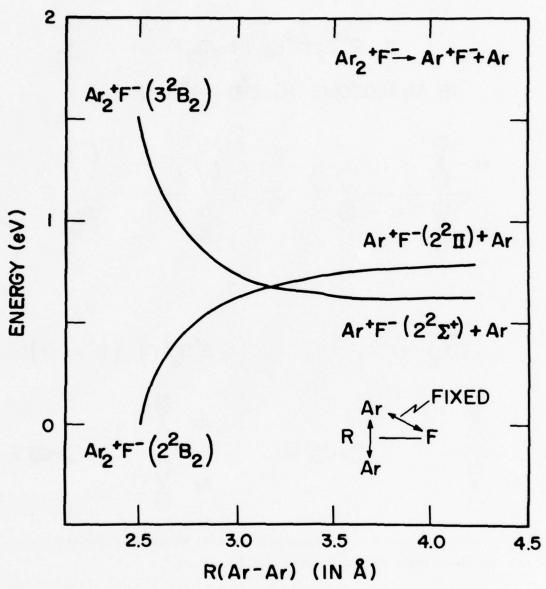
Graphical Data. A-9.2. Potential curves for ${\rm Ar}_2{\rm F}$ in an isosceles triangle configuration with the Ar-Ar distance fixed at 2.51 Å.



Graphical Data. A-9.3. Potential curves for $\mathrm{Ar}_2^{\,\mathrm{F}}$ in an isosceles triangle configuration with R_2 fixed at 2.25 Å.

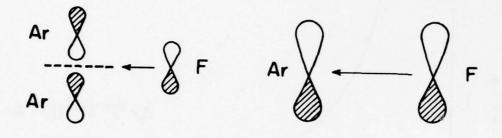


Graphical Data, A-9.4. Potential curves for Ar_2F in a collinear configuration varying both the Ar-Ar (bottom scale) and adjacent Ar-F (top scale) distances.



Graphical Data. A-9.5. Potential curves for the lowest two ionic states of ${\rm Ar}_2 {\rm F}$ in a right triangle configuration as a function of the Ar-Ar distance.

a. $2^2B_2^{-1}^2B_2^2 = 10^2B_2^2 = 10^2B_1^2 = 10^2$



b.

$$2^{2}B_{2} \rightarrow 1^{2}A_{1} \qquad (<2^{2}B_{2}|Y) (|1^{2}A_{1}>)$$

$$Ar \sqrt[8]{}$$

$$Ar \sqrt[8]{}$$

$$Ar \sqrt[8]{}$$

$$Ar \sqrt[8]{}$$

$$Ar \sqrt[8]{}$$

Graphical Data. A-9.6. Schematic orbital diagram of the two dipole-allowed emissions from the $2^2 \rm B_2$ state in $\rm Ar_2 F$.

Tabular Data. A-9.7. Estimate of the $2^2B_2 + 1^2B_2$ (1^2A_1) transition energy in Ar_2F and Kr_2F .

Arf $(2^2\Sigma^+-1^2\Sigma^+)$	$6.42 \text{ eV}^{\text{a}}$
$-D_e \left[\operatorname{Ar}_2^+(^2\Sigma_u^+) \right]$	-1.23 ^b
- Ar ₂ repulsion at Ar ₂ ($^2\Sigma_u^{+}$) R_e	-0.86°
Predicted Ar ₂ F $(2^2B_2 \rightarrow 1^2B_2, 1^2A_1)$	4.33 eV or 286 nm
$\operatorname{KrF} (2^2\Sigma^{\bullet} - 1^2\Sigma^{\bullet})$	5.00d
$-D_e \left[\operatorname{Kr}_2^+(^2\Sigma_u^+) \right]$	-1.15 ^b
- Kr_2 repulsion at $\operatorname{Kr}_2^+(^2\Sigma_u^+)R_e$	-0.86°
Predicted $Kr_2F(2^2B_2-1^2B_2, 1^2A_1)$	2.99 eV or 415 nm

^aJ. J. Ewing and C. A. Brau, Appl. Phys. Letts. <u>27</u>, 350 (1975)

^bC. Y. Ng., D. J. Trevor, B. H. Mahan, and Y. T. Lee, J. Chem. Phys. <u>66</u>, 446 (1977).

^cW. R. Wadt, J. Chem. Phys. <u>68</u>, 402 (1978).

dJ. M. Hoffman, A. K. Hays, and G. C. Tisone, Appl. Phys. Letts. 28, 538 (1976).

Tabular Data. A-9.8. Effect of F on the states of Ar_2 .

		Ar2F-	Ar_2^{\dagger}
$R_1(a_0)$	$R_2(a_0)$	$E(1^2A_2)-E(2^2B_2)(eV)$	$E(^2\Pi_g)-E(^2\Sigma_u^*)(\mathrm{eV})$
4.75	20.0	1,56	1.59
4.75	7.0	1.56	1,59
4.75	5.0	1.57	1.59
4.75	4.5	1.57	1.59
4.75	4.25	1.58	1.59
4.75	4.0	1.57	1,59
4.75		1.53	1,59
4,5	4.25	1.94	1,96
4.75	4.25	1.58	1.59
5.0	4.25	1.29	1.29
5.25	4.25	1.05	1,05
5.75	4.25	0.72	0.69
0.9	4,25	09.0	0.56

Tabular Data. A-9.9. Spectroscopic data for the 2^2B_2 ($4^2\Gamma$) state of Ar_2F with analogous data for the $2^2\Sigma^+$ [III(1/2)] state of ArF and the $1^2\Sigma^+$ [I(1/2)] state of Ar_2^+ without and with spin-orbit coupling.

	$\mathrm{Ar}_2\mathrm{F}(2^{2}B_2)$	$Ar_2F(2^2B_2)$ $ArF(2^2\Sigma^*)^a$	$\operatorname{Ar}_2^{+}(1^{}\Sigma_u^{+})^{\operatorname{b}}$
$R_e({ m Ar-F})({ m \AA})$	2.54	2.40	
$R_e({ m Ar-Ar})({ m \AA})$	2.48		2.50
$D_e(Ar_2^++F^-)(eV)$	2.00	5.52	
$D_e(Ar^+F^- + Ar)(eV)$	09.0		1.24
	$Ar_2F(4^2\Gamma)$	$ArF[III(1/2)]^a$	$\operatorname{Ar}_2^+[\operatorname{I}(1/2)_{\boldsymbol{u}}]^{\operatorname{b}}$
$D_e(Ar_2^++F^-)(eV)$	2,00	5.49	
$D_e({\rm Ar}^+{\rm F}^- + {\rm Ar})({\rm eV})$	0.57		1.19

^aT. H. Dunning and P. J. Hay, Chem. Phys. (in press).

b_W. R. Wadt. J. Chem. Phys. <u>68</u>, 402 (1978).

Tabular Data. A-9.10. Calculated data for the dipole-allowed emissions from the ${\bf 2}^2{\bf B}_2$ state of ${\rm Ar}_2{
m F}$ in its equilibrium isosceles triangle geometry neglecting spin-orbit effects.

	$\Delta E(eV)$	γ(nm)	M(D)	A (Sec-1)a
$2^2B_2 - 1^2A_1$	4.64	267	0.49	3.95×10 ⁶
$2^2B_2 \rightarrow 1^2B_2$	4.53	274	0.49	3.60×10^{6}

a The overall lifetime of the $2^2\mathrm{B}_2$ state is 132 nsec.

(including spin-orbit coupling) for the equilibrium isosceles triangle geometry Tabular Data. A-9.11. Transition moment (in a.u.) a from the 4 state of $\mathrm{Ar}_2\mathrm{F}$ of the 2^2B_2 state.

	$M_{\mathbf{x}}$	M_{y}	M_z	M
$4^2\Gamma - 1^2\Gamma$	5.09×10-4	1.92×10^{-1}	-4.12×10^{-2}	1.96×10-1
$4^2\Gamma - 2^2\Gamma$	1.43×10-4	1.66×10^{-2}	1.85×10^{-1}	1.86×10^{-1}
$4^2\Gamma - 3^2\Gamma$	5.98×10^{-4}	-1.29×10^{-2}	-2.75×10^{-2}	3.04×10^{-2}
$4^2\Gamma - 5^2\Gamma$	-6.04×10^{-3}	5.61×10^{-2}	$2.13{\times}10^{-2}$	6.03×10^{-2}
$4^2\Gamma - 6^2\Gamma$	-1.48×10^{-2}	-1.36×10-1	8.94×10^{-3}	1.37×10^{-1}
42r-72r	-5.14×10^{-5}	1.65×10-1	0	1.65×10-1
$4^2\Gamma - 8^2\Gamma$	9.72×10^{-5}	-4.12×10^{-2}	0	4.25×10 ⁻²
42r-92r	-4.60×10^{-3}	2.08	1.25×10-4	2.08

 a 1 e $_{0}$ = 2.541765 debye (D).

Tabular Data. A-9.12. Calculated data including spin-orbit coupling for the dipole-allowed emissions from the 4^Γ state of ${\rm Ar}_2 {\rm F}$ at the equilibrium isosceles triangle geometry of the $2^2 {\rm B}_2$ state.

	$\Delta E (eV)$	γ(nm)	M(D)	$A(sec^{-1})^a$
$4^2\Gamma - 1^2\Gamma$	4.64	267	0.50	4.08×10 ⁶
$4^2\Gamma - 2^2\Gamma$	4.52	274	0.47	3.40×10^{6}
$4^2\Gamma - 3^2\Gamma$	4.38	283	0.08	8.27×10^{4}

^aThe overall lifetime of the 4^2 state is 132 nsec.

Tabular Data. A-9.13. Calculated data for the dipole-allowed absorptions from ${\rm 2^2B_2}$ state of ${\rm Ar_2F}$ in its equilibrium isosceles triangle geometry neglecting spin-orbit effects.

	$\Delta E(eV)$	γ(nm)	M(D)	f
$2^2B_2 - 3^2B_2$	1.54	805	90.0	2.0×10-5
$2^2B_2-1^2A_2$	1.66	749	0.04	1.0×10 ⁻⁵
$2^2B_2-2^2A_1$	2.34	529	0.43	1.7×10^{-3}
$2^2B_2 - 3^2A_1$	3.88	320	5.29	0.41

Tabular Data. A-9.14. Calculated data for the dipole-allowed absorptions in ${\rm Ar}_2^+$ without $(^2\Sigma_{\bf u}^+)$ and with $[{\rm I}(1/2)_{\bf u}]$ spin-orbit coupling.

	$\Delta E (\mathrm{eV})$	γ(nm)	M(D)	f
$1^2\Sigma_u^+ - 1^2\Pi_g$	1.66	745	0.09	5.0×10^{-5}
$1^2\Sigma_u^+ - 1^2\Sigma_g^+$	3,89	319	5.26	0.41
$\mathrm{I}(1/2)_u \to \mathrm{I}(3/2)_g$	1,61	772	90.0	2.4×10^{-5}
$\mathrm{I}(1/2)_u \to \mathrm{I}(1/2)_g$	1.72	720	0.38	9.2×10-4
$\mathrm{I}(1/2)_{\boldsymbol{u}} \to \mathrm{II}(1/2)_{\boldsymbol{g}}$	3, 89	318	5.22	0.40

Tabular Data. A-9.15. Calculated data including spin-orbit coupling for the dipole-allowed absorptions from the $4^2\Gamma$ state of Ar $_2\Gamma$ at the equilibrium isosceles triangle geometry of the 2^2B_2 state.

	$\Delta E (eV)$	λ(nm)	M(D)	f
$4^2\Gamma \rightarrow 5^2\Gamma$	1.52	818	0.15	1.4×10 ⁻⁴
$4^2\Gamma \rightarrow 6^2\Gamma$	1.68	737	0.35	7.7×10^{-4}
$4^2\Gamma \rightarrow 7^2\Gamma$	2.33	531	0.42	1.6×10 ⁻³
$4^2\Gamma \rightarrow 8^2\Gamma$	2.58	481	0.11	1.1×10 ⁻⁴
$4^2\Gamma \rightarrow 9^2\Gamma$	3.88	319	5.29	0.41

Tabular Data. A-9.16. Spectroscopic data for the $2^2 B_2$ ($4^2 \Gamma$) state of Kr $_2F$ with analogous data for the $2^2 \Sigma^+$ [III(1/2)] state of Kr $_2F$ and the $1^2 \Sigma_u^+$ [(1/2) $_u$] state of Kr $_2^+$ without and with spin-orbit coupling.

	$Kr_2F(2^2B_2)$	$KrF(2^2\Sigma^+)^a$	$Kr_2^{\bullet}(1^2\Sigma_{\boldsymbol{u}}^{\bullet})^{b}$
$R_e(Kr-F)(\mathring{A})$	2.67	2.53	
$R_e(Kr-Kr)(\mathring{A})$	2.77		2.79
$D_e(\mathrm{Kr}_2^{\bullet}+\mathrm{F}^{-})(\mathrm{eV})$	4.95	5.36	
$D_e(\mathrm{Kr}^+\mathrm{F}^-+\mathrm{Kr})(\mathrm{eV})$	0.63		1.23
	$Kr_2F(4^2\Gamma)$	KrF[III(1/2)] ²	Kr ₂ *[I(1/2) _u] ^t
$D_e(\mathrm{Kr}_2^{\bullet} + \mathrm{F}^-)(\mathrm{eV})$	4.95	5.31	
$D_e(\mathrm{Kr}^+\mathrm{F}^-+\mathrm{Kr})(\mathrm{eV})$	0.49		1.05

^aP. J. Hay and T. H. Dunning, J. Chem. Phys. <u>66</u>, 1306 (1977).

^bW. R. Wadt. J. Chem. Phys. <u>68</u>, 402 (1978).

Tabular Data. A-9.17. Calculated data for the dipole-allowed emissions from $2^2 B_2$ state of Kr_2F in its equilibrium isosceles triangle geometry neglecting spin-orbit effects.

	ΔE (eV)	λ(nm)	M(D)	$A(\sec^{-1})^a$
$2^{2}B_{2} \rightarrow 1^{2}A_{1}$	3.47	357	0.66	2.97×10^6
$2^{2}B_{2} \leftarrow 1^{2}B_{2}$	3.38	368	0.85	4.61×10^6

 $^{^{\}mathrm{a}}$ The overall lifetime of the $\mathrm{2}^{2}\mathrm{B}_{2}$ state is 132 nsec.

Tabular Data. A-9.18. Transition moments (in a.u.) a from $4^2\Gamma$ state of $\mathrm{Kr}_2 F$ (including spin-orbit coupling) for the equilibrium isosceles triangle geometry of the $2^2 \mathrm{B}_2$ state.

	$M_{\mathbf{x}}$	M_{y}	M _z	M
$4^2\Gamma \rightarrow 1^2\Gamma$	1.2×10 ⁻³	2.59×10 ⁻¹	-1.24×10 ⁻¹	2.87×10 ⁻¹
$4^2\Gamma \rightarrow 2^2\Gamma$	5.22×10^{-4}	3.52×10^{-3}	3.13×10 ⁻¹	3.13×10 ⁻¹
$4^2\Gamma \rightarrow 3^2\Gamma$	3.51×10^{-3}	-1.26×10^{-2}	-4.81×10^{-2}	4.98×10 ⁻²
$4^2\Gamma \rightarrow 5^2\Gamma$	-1.63×10^{-2}	7.94×10^{-2}	4.20×10^{-2}	9.13×10 ⁻²
$4^2\Gamma \rightarrow 6^2\Gamma$	-2.11×10^{-2}	-6.18×10^{-1}	-3.29×10^{-2}	6.19×10 ⁻¹
$4^2\Gamma \rightarrow 7^2\Gamma$	-1.73×10^{-5}	1.53×10 ⁻¹	0	1.53×10 ⁻¹
$4^2\Gamma \rightarrow 8^2\Gamma$	1.01×10^{-4}	-9.30×10^{-2}	0	9.30×10^{-2}
$4^2\Gamma \rightarrow 9^2\Gamma$	-8.91×10^{-4}	2.12	-1.53×10^{-3}	2.12

 $a_1 ea_0 = 2.541765 \text{ debye (D)}.$

Tabular Data. A-9.19. Calculated data including spin-orbit coupling for the dipole-allowed emissions from the $4^2\Gamma$ state of $\mathrm{Kr}_2\Gamma$ at the equilibrium isosceles triangle geometry of the $2^2\mathrm{B}_2$ state.

	ΔE (eV)	λ(nm)	M(D)	$A(sec^{-1})^a$
$4^2\Gamma \rightarrow 1^2\Gamma$	3.44	361	0.73	3.55×10^{6}
$4^2\Gamma \rightarrow 2^2\Gamma$	3.34	371	0.80	$3.88{\times}10^6$
$4^2\Gamma \rightarrow 3^2\Gamma$	3.14	395	0.13	8.18×10^4

 $^{^{\}mathbf{a}}$ The overall lifetime of the $^{2}\Gamma$ state is 133 nsec.

Tabular Data. A-9.20. Calculated data for the dipole-allowed absorptions from $2^2 \mathrm{B}_2$ state of $\mathrm{Kr}_2 \mathrm{F}$ in its equilibrium isosceles triangle geometry neglecting the spin-orbit effects.

	$\Delta E (eV)$	λ(nm)	M(D)	f
$2^{2}B_2 \rightarrow 3^{2}B_2$	1.46	849	0.14	1.0×10-4
$2^{2}B_2 \rightarrow 1^{2}A_2$	1.56	794	0.07	2.8×10 ⁻⁵
$2^2B_2 \rightarrow 2^2B_1$	2.15	577	0.46	1.8×10 ⁻³
$2^{2}B_{2} \rightarrow 3^{2}A_{1}$	3.60	344	5.62	0.43

Tabular Data, A-9.21. Calculated data for the dipole-allowed absorptions in Kr_2^+ without $(^2\Sigma_{\mathbf{u}}^+)$ and with $[\mathrm{I(1/2)}_{\mathbf{u}}]$ spin-orbit coupling.

	$\Delta E (eV)$	$\lambda(nm)$	M(D)	f
$1^2 \Sigma_u^+ \rightarrow 1^2 \Pi_g$	1.57	790	0.15	1.3×10 ⁻⁴
$1^{2}\Sigma_{u}^{+} \rightarrow 1^{2}\Sigma_{g}^{+}$	3.59	346	5.39	0.40
$I(1/2)_u \rightarrow I(3/2)_g$	1.36	911	0.10	5.6×10 ⁻⁵
$\mathrm{I}(1/2)_u \to \mathrm{I}(1/2)_g$	1.75	708	1.55	1.6×10 ⁻²
$I(1/2)_u \rightarrow II(1/2)_g$	3.66	339	5.20	0.38

Tabular Data. A-9.22. Calculated data including spin-orbit coupling for the dipole-allowed absorptions from the $4^2\Gamma$ state of ${\rm Kr}_2 {\rm F}$ at the equilibrium isosceles triangle geometry of the $2^2 {\rm B}_2$ state.

	ΔE (eV)	λ(nm)	M(D)	f
$4^2\Gamma \rightarrow 5^2\Gamma$	1.32	938	0.23	2.7×10 ⁻⁴
$4^2\Gamma \rightarrow 6^2\Gamma$	1.73	718	1.57	1.6×10^{-2}
$4^2\Gamma \rightarrow 7^2\Gamma$	2.06	603	0.39	1.2×10^{-3}
$4^2\Gamma \rightarrow 8^2\Gamma$	2.59	478	0.24	5.2×10^{-4}
$4^2\Gamma \rightarrow 9^2\Gamma$	3.69	336	5.39	0.41

Tabular Data. A-9.23. Electronic state energies for ${\rm Ar_2F}$ and ${\rm Kr_2F}$ at their respective equilibrium isosceles triangle geometries without and with spin-orbit coupling. (Energies are in hartrees).

Without spin-orbit coupling		With spin-orbit coupling			
State	Ar_2F^a	Kr ₂ F ^b	State	Ar_2F^a	Kr ₂ F
$1^{2}A_{1}$	-0.89765	-0.13053	12Γ	-0.89777	-0.13066
$1^{2}B_{2}$	-0.89336	-0.12717	$2^2\Gamma$	-0.89337	-0.12713
$1^{2}B_{1}$	-0.88822	-0.11997	$3^2\Gamma$	-0.88810	-0.11988
2^2B_2	-0.72706	-0.00295	$4^2\Gamma$	-0.72716	-0.00439
$3^{2}B_{2}$	-0.67043	0.05070	$5^2\Gamma$	-0.67137	0.04418
$1^{2}A_{2}$	-0.66624	0.05443	$6^2\Gamma$	-0.66542	0.05907
2^2A_1	-0.64096	0.07596	$7^2\Gamma$	-0.64148	0.07117
2^2B_1	-0.63293	0.08467	$8^2\Gamma$	-0.63230	0.09090
3^2A_1	-0.58464	0.12934	$9^2\Gamma$	-0.58452	0,13123

^aEnergies are relative to -1152 hartree.

Tabular Data. A-9.24. The overall radiative life-time (in nsec) of the $2^2 \rm B_2$ state in $\rm Ar_2 F$ as a function of geometry. $\rm Ar_2 F$ has a $\rm C_{2v}$ isosceles triangle geometry with base = $\rm R_1$ and height = $\rm R_2$. $\rm R_1$ and $\rm R_2$ are in bohr (1a₀ = 0.529177 A).

R_1 R_2	4.0	4.25	4.5
4.5		222	
4.75	87.1	126	206
5.0		85.8	

 $^{^{}m b}$ Energies are relative to -5603 hartree.

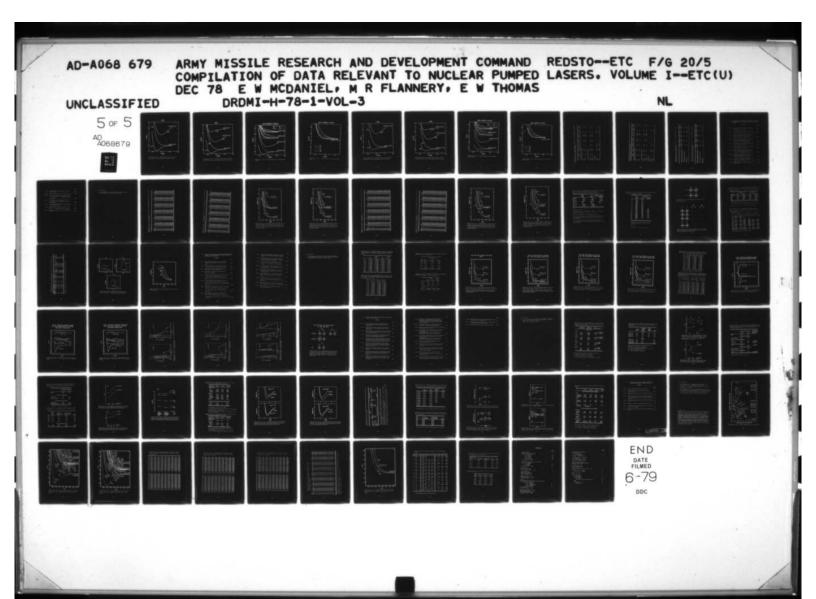
A-10. POTENTIAL ENERGY CURVES, SPECTROSCOPIC CONSTANTS, AND EMISSION DATA. FOR HgC ℓ and HgBr

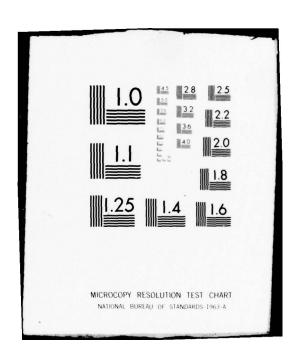
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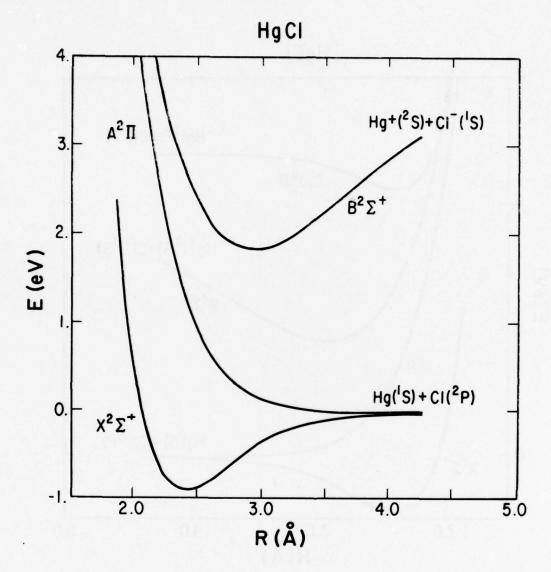
		Page
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A-10. References:

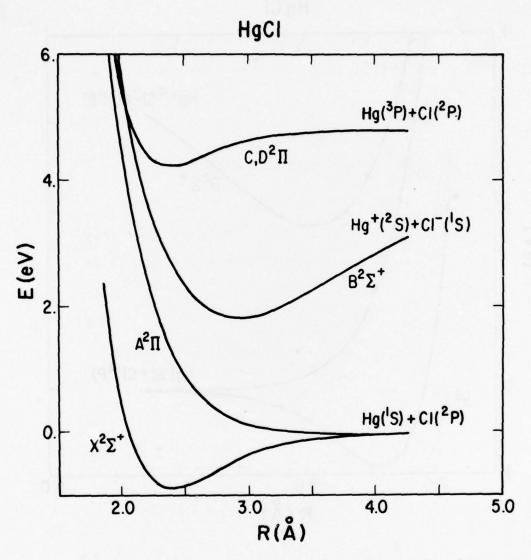
1. W. R. Wadt, "The Electronic Structure of HgC ℓ and HgBr," Appl. Letts. (in press).





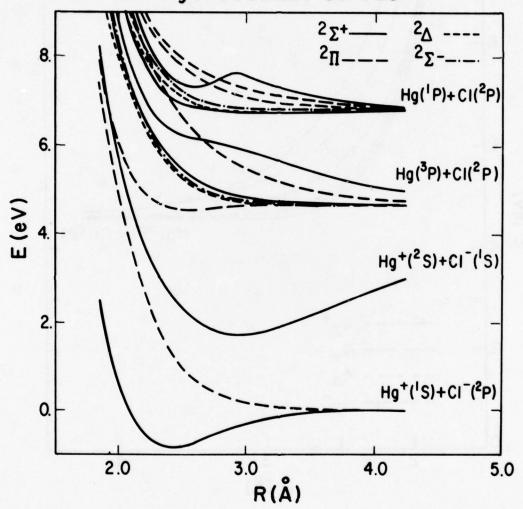


Graphical Data. A-10.1. Potential energy curves for the $X^2 \Sigma^+$, $A^2 \Pi$, and $B^2 \Sigma^+$ states of HgCl without spin-orbit coupling.

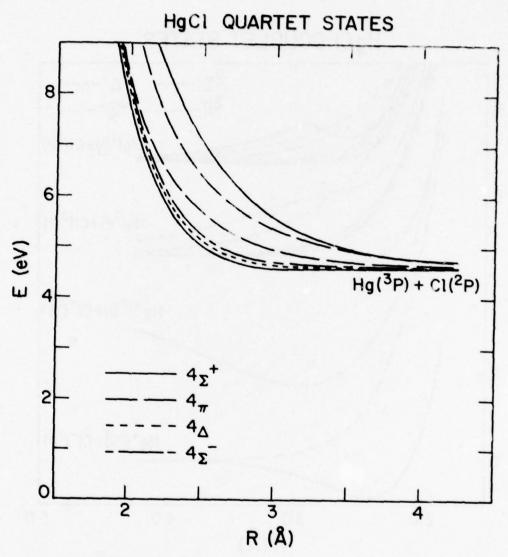


Graphical Data. A-10.2. Potential energy curves for the $X^2\Sigma^+$, $A^2\Pi$, $B^2\Sigma^+$, and $C,D^2\Pi$ states of HgCl without spin-orbit coupling.

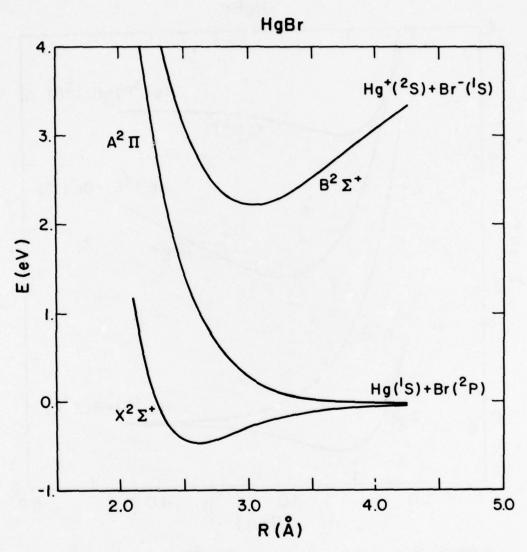
HgCI DOUBLET STATES



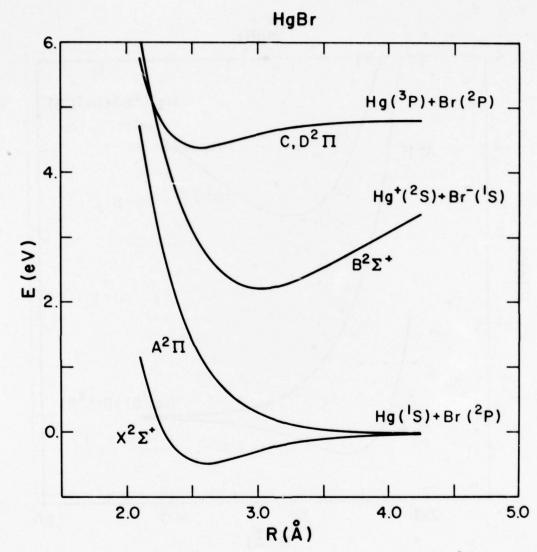
Graphical Data. A-10.3. Potential energy curves for ${\rm HgC}\ell$ doublet states.



Graphical Data. A-10.4. Potential energy curves for $\mathrm{HgC}\ell$ quartet states.

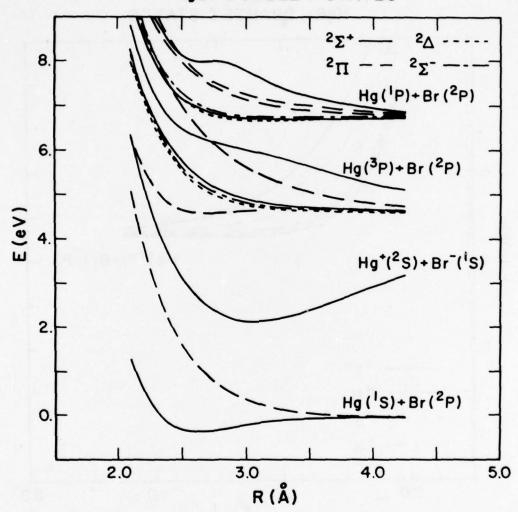


Graphical Data. A-10.5. Potential energy curves for the $X^2\Sigma^+$, $A^2\Pi$, and $B^2\Sigma^+$ states of HgBr without spin-orbit coupling.

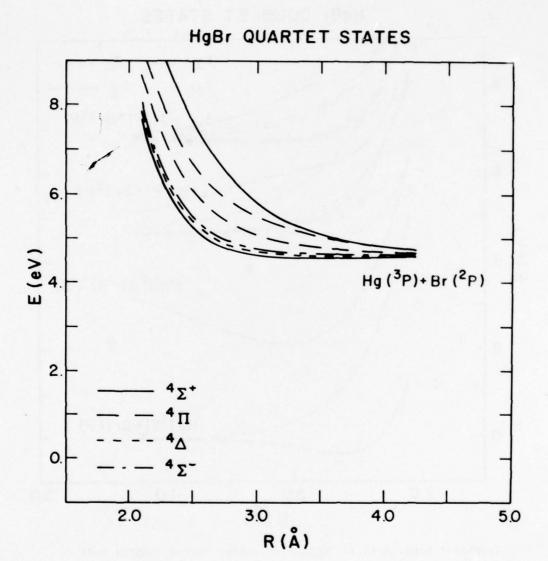


Graphical Data. A-10.6. Potential energy curves for the $X^2\Sigma^+$, $A^2\Pi$, $B^2\Sigma^+$, and C, $D^2\Pi$ states of HgBr without spin-orbit coupling.

HgBr DOUBLET STATES



Graphical Data. A-10.7. Potential energy curves for the HgBr doublet states.



Graphical Data. A-10.8. Potential energy curves for the ${\tt HgBr}$ quartet states.

Tabular Data. A-10.9. Spectroscopic constants for the X and B states of $\rm Hg$ $_{\rm Cl}^{35}$ with and without spin-orbit coupling.

Spin-Orbit Coupling 2.41		R (A)	$e_{e(cm^{-1})} \frac{x_{e}_{e(cm^{-1})} B_{e(cm^{-1})}}{e^{(cm^{-1})}}$	x w (cm) B (cm 1)	a (cm 1)	2 (eV)	n(0)1
2.41 285.3 2.25 .098 2.93 198.8 .51 .066 Spin-Orbit Coupling /2 2.42 285.6 2.29 .098 /2 2.93 198.0 .56 .066 sriment /2 — 292.6 1.60 — 192.0 .50 —	Without	Spin-Orbi	t Coupling					
2.93 198.8 .51 .066 In-Orbit Coupling 2.42 285.6 2.29 .098 2.93 198.0 .56 .066 - 292.6 1.60 192.0 .50	x ² z ⁺	2.41	285.3	2.25	860.	92000.	.91	3.28
1n-Orbit Coupling 2.42 285.6 2.29 .098 2.93 198.0 .56 .066	B ² 2+	2.93	198.8	.51	990.	.00015	4.77	5.41
2.42 285.6 2.29 .098 2.93 198.0 .56 .066 ant 292.6 1.60 192.0 .50	With Sp.	in-Orbit C	Coupling					
2.93 198.0 .56 .066 ent 292.6 1.60 192.0 .50	$x^2z_{1/2}^+$	2.42	285.6	2.29	860.	7.00077	.87	3.28
ent — 292.6 1.60 — — — — — — — — — — — — — — — — — — —	$B^2_{\Sigma_{1/2}}$		198.0	. 56	990.	.00015	4.77	5.41
- 292.6 1.60 - - 192.0 .50	Experim	ent						
- 192.0 .50	$x^2_{\Sigma_{1/2}^+}$	1	292.6	1.60	1	1	1.08	١
	B ² E	1	192.0	.50	1	1	66.4	1

	R _e (A)	w (cm -1)	x m (cm 1) B (cm 1)	B (cm -1)	$\alpha_{\rm e}({\rm cm}^{-1})$	D _e (eV)	n(D)
Without	Spin-Orbi	Without Spin-Orbit Coupling					
x ² E ⁺	2.61	159.4	1.64	0.044	07000.	.48	2.62
B ² E ⁺	3.04	141.8	.29	.032	90000.	4.77	5.51
With Sp:	With Spin-Orbit Coupling	coupling					
x^2 _{1/2}	2.62	159.4	1.64	770.	77000.	.33	2.62
${_{\rm B}}^2\Sigma_{1/2}^+$	3.05	141.8	.29	.032	90000.	4.77	5.51
Experiment	ent						
$x^2 \varepsilon_{1/2}^+$	1	186.5	.97	ı	ı	.71	١
B22+1/2	١	135.1	.28	ı	1	4.87	1

Tabular Data. A-10.11. Emission data for the B \rightarrow X lasing transition in HgCl with and without spin-orbit coupling.

	T _e (eV)	$T_e(eV)$ $\Delta E(eV)$ $\lambda(nm)$ $M(D)$) (nm)	M(D)	T(ns)
Without Spin-Orbit Coupling	2.73	2.73 2.25 552 4.37	552	4.37	27.4
With Spin-Orbit Coupling	2.73	2.25	552	4.36	27.5
Experiment	2.90	2.22	558	3.52	9.47
				66.7	22.2

Tabular Data. A-10.12. Emission data for the B $\,\div$ X lasing transition in HgBr with and without spin-orbit coupling.

	Te (eV)	$T_{e}(eV)$ $\Delta E(eV)$ $\lambda(nm)$ $M(D)$ $\tau(ns)$	γ(nm)	M(D)	t(ns)
Without Spin-Orbit Coupling	2.70	2.70 2.50	497 3.88 26.0	3.88	26.0
With Spin-Orbit Coupling	2.70	2.50	167	3.77 27.6	27.6
Experiment	2.91	2.47	502	4.12 23.7	23.7

A-11. POTENTIAL ENERGY CURVES, ELECTRONIC ENERGIES, SPECTROSCOPIC CONSTANTS, AND DIPOLE AND TRANSITION MOMENTS FOR THE RARE GAS OXIDES

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A-11. References:

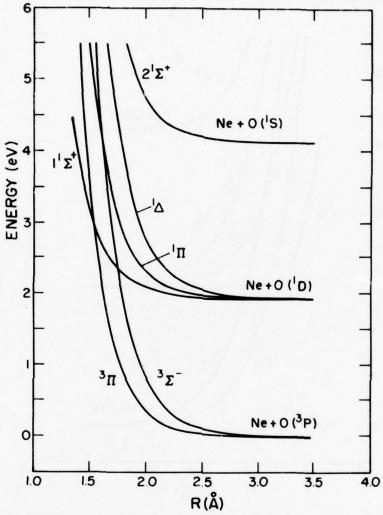
1. T. H. Dunning and P. J. Hay, "Low-Lying Electronic Data of the Rare-Gas Oxides," J. Chem. Phys. <u>66</u>, 3767 (1977).

Tabular Data. A-11.1 Total energies of the states of NeO arising from Ne $^{(1)}$ S) + 0 $^{(3)}$ P, $^{(1)}$ D, $^{(1)}$ S). Energies are relative to -203 hartree.

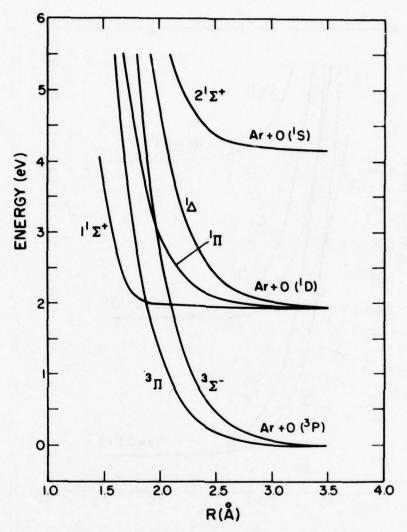
$R(a_0)$	Π^{ϵ}	32-	$1^{1}\Sigma^{\bullet}$	п	۵,	2 1 Z*
2.50	-0.10974	0.07731	-0.19091	-0.03497	0.15266	0.20825
2,75	-0.22077	-0.10267	-0.23476	-0.14415	-0.02472	0.03748
3.00	-0.28369	-0.20963	-0.25589	-0.20469	-0.12986	-0.06148
3, 25	-0.31950	-0.27310	-0.26673	-0.23847	-0.19217	-0.11767
3.50	-0,33990	-0.31077	-0.27304	-0.25750	-0.22909	-0.14886
3,75	-0.35145	-0.33308	-0.27701	-0.26827	-0.25091	-0.16589
4.00	-0.35792	-0.34626	-0.27946	-0.27438	-0.26377	-0.17516
4.25	-0.36151	-0.35402	-0.28088	-0.27782	-0.27133	-0.18026
4.50	-0.36347	-0.35859	-0.28165	-0.27976	-0.27577	-0.18309
5.00	-0.36508	-0.36283	-0.28219	-0.28141	-0.27987	-0.18556
5.50	-0.36546	-0.36424	-0.28223	-0.28185	-0.28123	-0.18631
6.00	-0.36550	-0.36467	-0.28215	-0.28191	-0.28164	-0.18649
7.00	-0.36542	-0.36475	-0.28203	-0.28184	-0.28172	-0.18647
8.50	-0.36539	-0.36473	-0.28199	-0.28181	-0.28169	-0.18644
12,00	-0.36539	-0.36472	-0.28198	-0.28180	-0.28169	-0.18644

Tabular Data. A-11.2. Total energies of the states of ArO arising from Ar $(^1$ S) + 0 $(^3$ P, 1 D, 1 S). Energies are relative to -601 hartree.

$R(a_0)$	311	3 _Σ -	112.	1,	ړ. م	212
2,75	-0.29182	-0.06217	-0.44208	-0.24285	-0.00417	0,03161
2.875	-0.35262	-0.15344	-0.46954	-0.30044	-0.09150	-0.05269
3.00	-0.40244	-0.23193	-0.48830	-0.34717	-0,16622	-0.12417
3.25	-0.47548	-0.35453	-0.50857	-0.41414	-0.28227	-0.23285
3.50	-0.52268	-0.43958	-0.51604	-0,45558	-0.36285	-0.30585
3,75	-0.55285	-0.49694	-0.51786	-0.48064	-0.41755	-0.35331
4.00	-0.57201	-0.53483	-0.51800	-0.49573	-0.45394	-0.38287
4.25	-0.58409	-0.55947	-0.51812	-0.50489	-0.47773	-0.40042
4.50	-0.59159	-0.57528	-0.51848	-0.51050	-0.49304	-0.41045
5.00	-0.59896	-0.59165	-0.51924	-0.51607	-0.50894	-0.41932
5.50	-0.60156	-0.59812	-0.51953	-0.51815	-0.51521	-0.42227
6.00	-0.60241	-0.60062	-0.51952	-0.51886	-0.51763	-0.42328
6.50	-0.60261	-0.60152	-0.51940	-0.51904	-0.51850	-0.42359
7.00	-0.60260	-0.60178	-0.51927	-0.51902	-0.51875	-0.42362
8.50	-0.60247	-0.60180	-0.51907	-0.51889	-0.51876	-0.42352
12.00	-0.60245	-0.60178	-0.51905	-0.51887	-0.51875	-0.42350



Graphical Data. A-11.3. Calculated potential energy curves for the states of NeO arising from the Ne (^1S) + 0 $(^3P$, 1D , $^1S)$ separated atom limits. The curves have been uniformly shifted to correct for the errors in the 0 $(^1D$ - $^3P)$ and 0 $(^1S$ - $^3P)$ excitation energies.



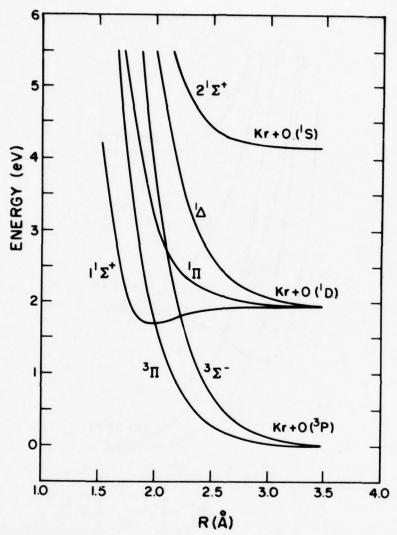
Graphical Data. A-11.4. Calculated potential energy curves for the states of ArO arising from the Ar (^1S) + 0 $(^3P, ^1D, ^1S)$ separated atom limits. The curves have been uniformly shifted to correct for the errors in the 0 $(^1D - ^3P)$ and 0 $(^1S - ^3P)$ excitation energies.

Tabular Data. A-11.5. Total energies of the states of KrO arising from Kr $(^1$ S) + 0 $(^3$ P, 1 D, 1 S). Energies are relative to -2826 hartree.

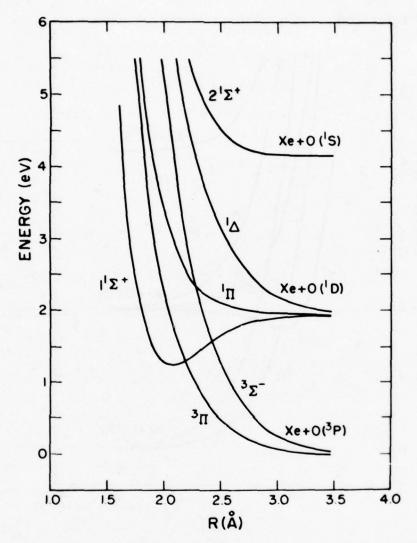
$R(a_0)$	Π_{ϵ}	32-	112.	П	Δ,	212
2.875	-0.40859	-0.19828	-0.55182	-0.36789	-0.14745	-0.11674
3.00	-0.46706	-0.27803	-0.58546	-0.42315	-0.22337	-0.19086
3,125	-0.51513	-0.34767	-0.60858	-0.46801	-0.28906	-0.25437
3.25	-0.55449	-0.40802	-0.62400	-0.50422	-0.34548	-0.30813
3,375	-0.58656	-0.45990	-0.63382	-0.53318	-0.39359	-0.35311
3.50	-0.61252	-0.50418	-0.63955	-0.55604	-0.43439	-0.39033
3.75	-0.65040	-0.57327	-0.64338	-0.58776	-0.49801	-0.44611
4.00	-0.67496	-0.62156	-0.64207	-0.60655	-0.54289	-0.48311
4.25	-0.69085	-0.65452	-0.63947	-0.61754	-0.57393	-0.50673
4.50	-0.70106	-0.67656	-0.63736	-0.62403	-0.59493	-0.52092
4.75	-0.70756	-0.69107	-0.63612	-0.62794	-0.60886	-0.52892
5.00	-0.71164	-0.70050	-0.63552	-0,63036	-0.61796	-0.53329
5.50	-0.71572	-0.71049	-0.63508	-0.63284	-0.62764	-0.53701
00.9	-0.71719	-0.71457	-0.63487	-0.63381	-0.63160	-0.53825
6.50	-0.71765	-0.71619	-0.63467	-0.63413	-0.63317	-0.53867
2.00	-0.71773	-0.71676	-0.63449	-0.63417	-0.63372	-0.53876
8.50	-0.71757	-0.71689	-0.63418	-0.63399	-0.63386	-0.53862
12.00	-0.71753	-0.71686	-0.63413	-0.63394	-0.63383	-0.53858

Tabular Data. A-11.6. Total energies of the states of XeO arising from Xe (^1S) + 0 $(^3P, ^1D, ^1S)$. Energies are relative to -7306 hartree.

$R(a_0)$	Π^{ϵ}	32-	112.	П1	η.	212
3.00	-0.31839	-0.14551	-0.44467	-0.28890	-0.10619	-0.08134
3, 125	-0.37811	-0.21500	-0.49122	-0.34653	-0.17279	-0.14771
3,25	-0.42548	-0.27347	-0.52356	-0.39120	-0.22770	-0.20198
3,375	-0.46388	-0.32392	-0.54568	-0.42648	-0.27416	-0.24731
3.50	-0.49542	-0.36797	-0.56045	-0.45476	-0.31415	-0.28579
3,625	-0.52136	-0.40656	-0.56975	-0.47748	-0.34875	-0.31852
3.75	-0.54255	-0.44043	-0.57481	-0.49545	-0.37858	-0.34592
4.00	-0.57376	-0.49605	-0.57659	-0.52010	-0.42645	-0.38701
4.25	-0.59438	-0.53783	-0.57246	-0.53405	-0.46238	-0.41435
4.50	-0.60812	-0.56823	-0.56659	-0.54156	-0.48927	-0.43243
4.75	-0.61736	-0.58972	-0,56128	-0.54550	-0.50888	-0.44388
5.00	-0.62355	-0.60457	-0.55744	-0.54762	-0.52275	-0.45039
5.25	-0.62767	-0.61467	-0,55506	-0.54887	-0.53231	-0.45362
5.50	-0.63037	-0.62143	-0.55370	-0.54969	-0.53878	-0.45500
6.00	-0.63323	-0.62888	-0.55250	-0.55065	-0.54596	-0.45576
6.50	-0.63434	-0.63208	-0.55203	-0.55110	-0.54907	-0.45591
7.00	-0.63474	-0.63340	-0.55179	-0.55128	-0.55037	-0.45596
8.50	-0.63481	-0.63411	-0.55144	-0.55124	-0.55107	-0.45587
12.00	-0.63474	-0.63407	-0.55134	-0.55116	-0.55104	-0.45579



Graphical Data. A-11.7. Calculated potential energy curves for the states of KrO arising from the Kr (^1S) + 0 $(^3P$, 1D , 1S) separated atom limits. The curves have been uniformly shifted to correct for the errors in the 0 $(^1D$ - 3P) and 0 $(^1S$ - 3P) excitation energies.



Graphical Data. A-11.8. Calculated potential energy curves for the states of XeO arising from the Xe (^1S) + 0 $(^3P$, 1D , $^1S)$ separated atom limits. The curves have been uniformly shifted to correct for the errors in the O $(^1D$ - $^3P)$ and O $(^1S$ - $^3P)$ excitation energies.

Tabular Data. A-11.9. Calculated spectroscopic constants for the 1^{1} states of 84 Kr 16 O and 132 Xe 16 O. Units are as indicated.

	KrO	X	eO
	Calc	Calc	Exptl a,t
Te, eVe	1.71	1.26	1.60
Re, Å	2.00	2.08	2.65
De, eV	0.25	0.70	0.36
ω_e , cm ⁻¹	375d	470 ^d	372
	12	6.6	12
B_e , cm ⁻¹	0.317	0.275°	
α_e	0.011	0.0045	

^aReferences 1, A-11.

^bFor a discussion of the "experimental" constants of the 1^1E^+ state of XeO, see A-11 Ref. 1.

^cRelative to the Rg $(^{1}S) + 0$ (^{3}P) separated atom limit.

 $^{^{}m d}$ The calculated w_e and $w_e x_e$ were obtained from a least-squares fit of the lowest 8 (KrO) or 16 (XeO) vibrational energies with a four term expansion.

^eThe calculated B_c and α_c were obtained from a least-squares fit of the lowest 8 (KrO) or 16 (XeO) rotation constants (B_c) with a four term expansion.

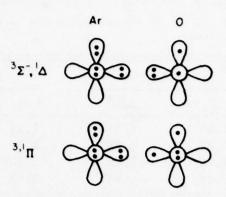
Tabular Data. A-11.10. Vibrational levels and spacings for the $1^{1}\Sigma^{+}$ state of XeO. Energies are in cm⁻¹.

	G(v)	ΔG	$(v+\frac{1}{2})$
υ	Calca	Calc	Exptl ^b
0	232	457	
1	690	44	
2	1134	431	
3	1565	416	
4	1981	401	
5	2382	385	
6	2767	367	
7	3134	349	347
8	3483	328	328
9	3811	306	302
10	4118	282	272
11	4400	256	252
12	4656	226	224
13	4882	193	201
14	5075	158	186
15	5233		200

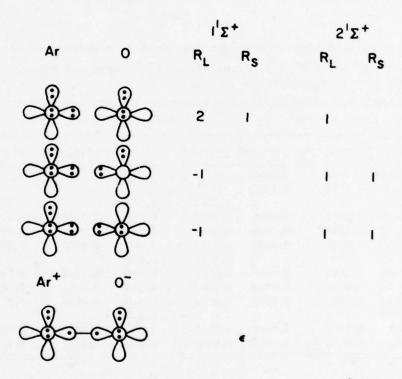
^aObtained by solving the vibrational (J = 0) Schroedinger equation with the calculated potential.

b_{Reference 1.}

^cSeven higher levels are omitted here.



Graphical Data. A-11.11. Orbital diagrams for the $^{3,1}{\rm R}$ and $^{3}{\rm E}^{-}$, and $^{1}{\rm A}$ states of ArO .



Graphical Data. A-11.12. Orbital diagrams for the 1,2 $^1\Sigma^+$ states of ArO. Configuration coefficients (unnormalized) for both large R(R_L) and short R(R_S) have been listed.

Tabular Data. A-11.13. Calculated crossing points and energies for the $1^1\Sigma^+$ - $^3\Pi$ and $1^1\Sigma^+$ - $^3\Sigma^-$ crossings in the rare gas monoxides. Units are as indicated.

	$1^{1}\Sigma^{+}-^{3}\Pi$		$1^{1}\Sigma^{+}-^{3}\Sigma^{-}$	
Molecule	R_c	$\Delta E_c^{\ b}$	R_c	$\Delta E_c^{\ b}$
NeO	1.53 Å	0.92 eV	1.74 Å	0.39 eV
ArO	1.87	0.068	2.09	0.028
KrO	2.00	-0.25	2.23	-0.16
XeO	2.19	-0.64	2.42	-0.37

^aThe curves have been shifted to correct for the error in the calculated 0 (1 D) - 0 (3 P) excitation energy; see A-11 Ref. 1.

Tabular Data. A-11.14. Calculated transition moments for the $2^1 \Sigma^+ - 1^1 \Sigma^+$ and $2^1 \Sigma^+ - 1^1 \Pi$ transitions in the rare gas monoxides. Moments are in atomic units.

	Are	0	K	rO	Xe	90
R (a ₀)	2 ¹ Σ*-1 ¹ Σ*	2 1Σ*-111 a	2 ¹ Σ*-1 ¹ Σ*	21Σ·-111 a	2 15 -1 15 +	2 1Σ*-1Π°
2.75	0.0099	0.1273				
3.00	0.1847	0.1062				
3.25			0.2165	0.0835		
3.50	0.3512	0.0819	0.3123	0.0894	0,2165	0.0584
4.00	0.3862	0.0598	0.4951	0.0880	0.4093	0.1211
4.50	0.2703	0,3091	0.4890	0.0704	0.6723	0.0822
4.75			0.4132	0.0590		
5.00	0.1464	0.0236	0.3233	0.0480	0.7033	0.0468
5.50	0.0690	0.0142	0.1762	0.0305	0.4784	0.0253
6.00	0.0403	0.0089	0.0886	0.0196	0.2628	0.0146
6.50				0.0132		
7.00	0.0403	0.0089	0.0287		0.0728	0.0063
8.50	0.0043	0.0019	0.0085	0.0041	0.0167	0.0027

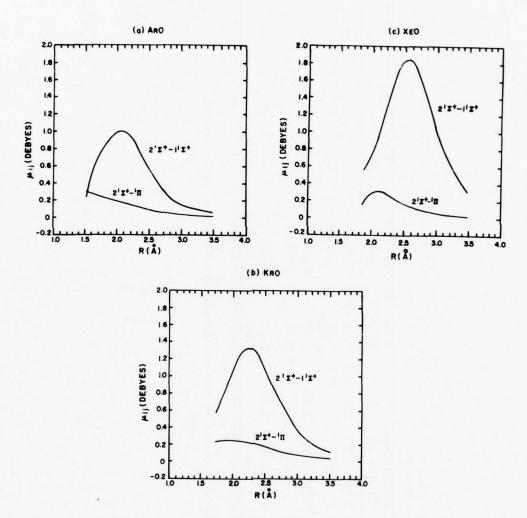
^aThe matrix element given is $\left\langle 2^{1} \Sigma^{+} |\chi|^{1} \Pi_{\chi} \right\rangle$.

 $^{^{}b}$ Relative to the Rg $(^{1}$ S) + 0 $(^{1}$ D) separated atom energy.

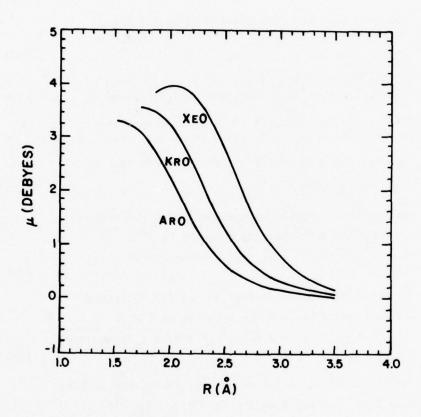
Tabular Data. A-11.15. Calculated pseudo-lifetimes for the $2^{1\Sigma}^+$ states of the rare gas oxides. Units are as indicated.

Molecule	Transition	R*	$\Delta E(R^*)^2$	$\mu_{ij}(R^*)$	$A_{ ho}$	Tp
ArO	2 ¹ Σ*-1 ¹ Σ* - ¹ Π	2.97 Å	2.26 eV 2.22	0.0598 ea ₀ 0.0128	$4.4 \times 10^4 \text{ sec}^{-1}$ 4.4×10^3	23 μsec 230
KrO	$2^{1}\Sigma^{\bullet}-1^{1}\Sigma^{\bullet}$ -1Π	3.02	2.27	0.134 0.0254	2.2×10^5 1. 7×10^4	4.5 60
Xe0	$2^{1}\Sigma^{+}_{1}^{1}\Sigma^{+}_{1}$ $-^{1}\Pi$	2.89	2.32	0.496 0.0264	3.3×10^{6} 1.6×10^{4}	0.31 62

^a Corrected for the error in the calculated $0(^{1}S)-0(^{1}D)$ excitation energy.



Graphical Data. A-11.16. Dipole transition moments for the $2^1\Sigma^+$ - $1^1\Sigma^+$ and $2^1\Sigma^+$ - 1^1 transitions in ArO, KrO and XeO.



Graphical Data. A-11.17. Dipole moments for the $1^1\Sigma^+$ states of ArO, KrO, and XeO.

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A-12. References:

1. T. H. Dunning, M. Valley, and H. S. Taylor, "Theoretical Studies of the Low-Lying Electronic States of GaKr, Including Extrapolation to InKr and T ℓ Kr," J. Chem. Phys. <u>69</u>, 2672 (1978).

Tabular Data. A-12.1. Energies obtained from the POL-CI calculations on the low-lying electronic states of GaKr and $GaKr^+$. Distances are in bohr; energies are in hartree. Energies are relative to -4674 hartree.

R	1 ² Π	GaKr 1 ² Σ*	2 ² ∑ *	GaKr*
3.75	-1.02539	- 0.96866	-0.93379	- 0.85625
4.00	-1.07933	-1.01870	-0.99238	-0.90683
4.50	-1.14810	-1.08688	-1.06440	- 0.96758
5.00	-1.17924	-1.13516	-1.08855	-0.99287
5.50	-1.19225	-1.16324	-1.09545	-1.00070
6.00	-1.19772	-1.17938	-1.09677	-1.00202
6.50	-1.19984	-1.18865	-1.09631	-1.00107
7.00	-1.20045	-1.19396	-1.09545	-0.99950
8.00	-1.20020	-1.19865	-1.09420	-0.99670
0.00	-1.19933	-1.20029	-1.09406	-0.99402
15.00	-1.19878	-1.20012	-1.09502	-0.99304

Tapular Data. A-12.2. Calculated energies of the I 1/2, II 1/2, and I 3/2 states of GaKr with spin-orbit corrections. Distances are in bohr; energies are in hartree. Energies are relative to the energy of the $1^2\Sigma^+$ state at R = 15 a_0 .

R	I 1/2	I 3/2	II 1/2
3.75	0.17228	0.17484	0.23152
4.00	0.11835	0.12091	0.18147
4.50	0.04957	0.05213	0.11329
5.00	0.01841	0.02099	0.06502
5.50	0.00538	0.00799	0.03698
6.00	-0.00015	0.00252	0.02089
6.50	-0.00234	0.00040	0.01170
7.00	-0.00307	-0.00022	0.00650
8.00	-0.00316	0.00003	0.00215
10.00	-0.00280	0.00090	0.00103
15.00	-0.00251	0.00126	0.00126

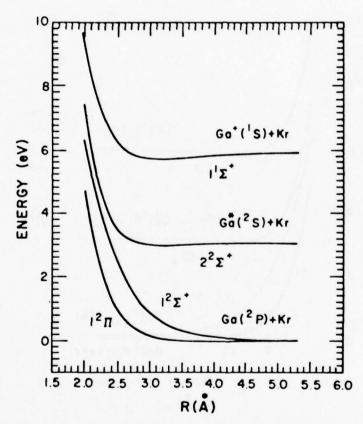
Tabular Data. A-12.3. Excitation energies and ionization potentials for the Ga, In, and T1 atoms, in ${\rm eV}$.

Group IIIA atoms				
State	Ga	ln	Tl	
$^{2}P_{1/2}$	0.000	0.000	0.000	
² P _{3/2}	0.102	0.274	0.966	
² S _{1/?}	3.073	3.022	3.282	
¹ S ₀	5.998	5.786	6.108	

Tabular Data. A-12.4. Spectroscopic constants for the bound states of $^{69}\mathrm{Ga}^{84}\mathrm{Kr}$ and $^{69}\mathrm{Ga}^{84}\mathrm{Kr}^+$. Units are as indicated.

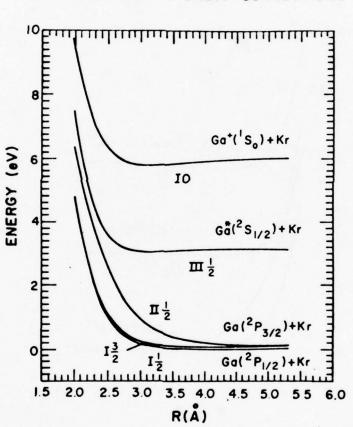
	Ga	GaKr*	
	1 ² Π	5;2.	1,52,
T_e , eV	0.00	2.82	5.40
Re, Å	3.78	3.17	3.14
D_e , eV	0.041	0.047	0.24
ω _e , cm ⁻¹	36	66	83
B_e	0.0312	0.0442	0.0452

THE LOW-LYING STATES OF GoKr AND GoKr+



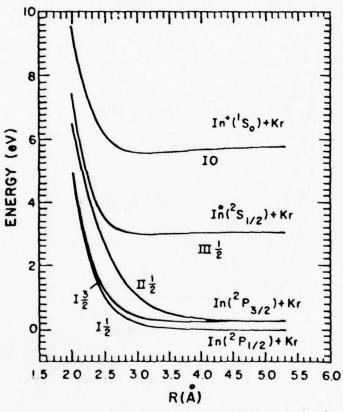
Graphical Data. A-12.5. Calculated potential energy curves for the states of GaKr and GaKr $^+$ arising from the Ga (2 P, 2 S) + Kr (1 S) and Ga $^+$ (1 S) + Kr (1 S) separated atom limits. The curves have been uniformly shifted to correct for the errors in the gallium atom excitation energies.

THE LOW-LYING STATES OF Gakr AND Gakr * WITH SPIN-ORBIT CORRECTIONS



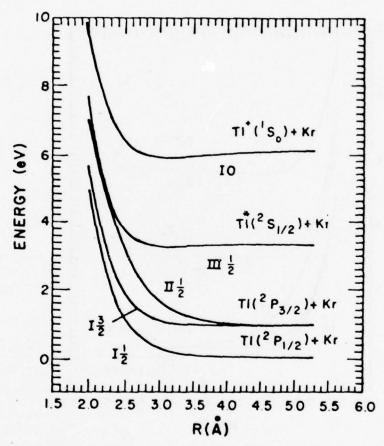
Graphical Data. A-12.6. Calculated potential energy curves for the states of GaKr and GaKr⁺ arising from the Ga (2 P $_{1/2}$, $_{3/2}$, 2 S $_{1/2}$) + Kr (1 S $_0$) and Ga⁺ (1 S $_0$) + Kr (1 S $_0$) separated atom limits. The curves have been uniformly shifted to correct for the errors in the gallium excitation energies.

THE LOW-LYING STATES OF INK AND INK WITH SPIN-ORBIT CORRECTIONS



Graphical Data. A-12.7. Model potential energy curves for the states of InKr and InKr $^+$ arising from the In (2 P $_1/2$, 3/2, + Kr (1 S $_0$) and In $^+$ (1 S $_0$) + Kr (1 S $_0$) separated atom limits.

THE LOW-LYING STATES OF TIKE AND TIKE WITH SPIN-ORBIT CORRECTIONS



Graphical Data. A-12.8. Model potential energy curves for the states of T1Kr and T1Kr $^+$ arising from the T1 (2 P $_{1/2}$, 3/2, 2 S $_{1/2}$) + Kr (1 S $_0$) and In $^+$ (1 S $_0$) + Kr (1 S $_0$) separated atom limits.

Tabular Data. A-12.9. Dipole transition moments coupling the low-lying states of GaKr obtained from the POL-C1 calculations.

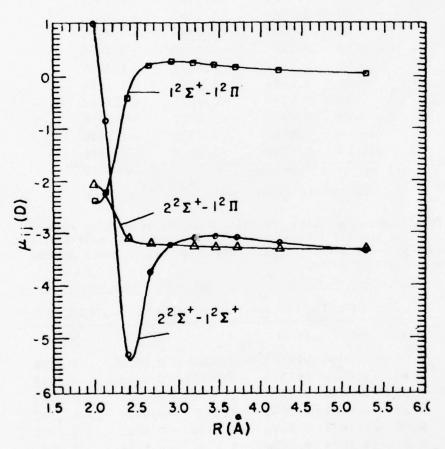
R	$1^{2}\Sigma^{4}-1^{2}\Pi^{a}$	$2^{2}\Sigma^{4}-1^{2}\Pi^{a}$	$2^2\Sigma^*-1^2\Sigma^*$
3.75	- 0.9037	-0.7877	0.4095
4.00	-0.8462	-0.8680	-0.3055
4.50	-0.1365	-1.2090	-2.0676
5.00	0.0992	-1.2349	-1.4402
5.50	0.1257	-1.2469	-1.2456
6.00	0.1166	-1.2554	-1.1893
6.50	0.0984	-1.2619	-1.1800
7.00	0.0789	-1.2677	-1.1902
8.00	0.0476	-1.2777	-1.2310
10.00	0.0163	-1.2898	-1.2976
15.00	0.0018	-1.2917	-1.3101

^aThe matrix element given is $\langle n^2 \Sigma^+ | \chi | 1^2 \pi_{\chi} \rangle$.

Tabular Data. A-12.10. Calculated dipole transition moments coupling the III 1/2 and I 1/2, II 1/2 and I 3/2 states of GaKr with spin-orbit corrections. Distances are in bohr; moments are in atomic units.

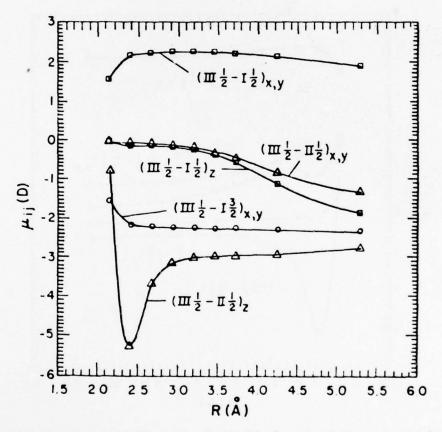
	III 1/2-	-I 1/2	III 1/2-	-II 1/2	III 1/2-I 3/2
R	Z	(x, y)	Z	(x,y)	(x, y)
4.00	-0.0086	0.6135	-0.3054	-0.0173	-0.6138
4.50	-0.0576	0.8545	-2.0667	-0.0238	-0.8549
5.00	-0.0549	0.8726	-1.4392	-0.0333	-0.8732
5.50	-0.0701	0.3803	-1.2437	-0.0496	-0.8817
6.00	-0.1007	0.8845	-1.1850	-0.0752	-0.8877
6.50	-0.1504	0.8850	-1.1704	-0.1138	-0.8923
7.00	-0.2249	0.8803	-1.1688	-0.1694	-0.8964
8.00	-0.4405	0.8436	-1.1495	-0.3233	-0.9035
10.00	-0.7254	0.7562	-1.0759	-0.5098	-0.9120
15.00	-0.7564	0.7457	-1.0697	-0.5273	-0.9134

DIPOLE TRANSITION MOMENTS AMONG THE LOW-LYING STATES OF Gakr



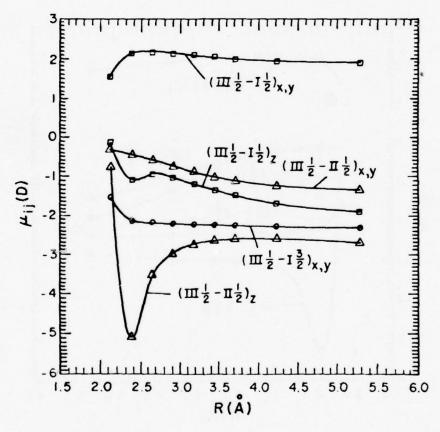
Graphical Data. A-12.11. Calculated dipole transition moments for $1^2\Sigma^+ - 1^2\Pi$, $2^2\Sigma^+ - 1^2\Pi$, and $2^2\Sigma^+ - 1^2\Sigma^+$ transitions in GaKr.

DIPOLE TRANSITION MOMENTS AMONG THE LOW-LYING STATES OF Gakr WITH SPIN-ORBIT CORRECTIONS

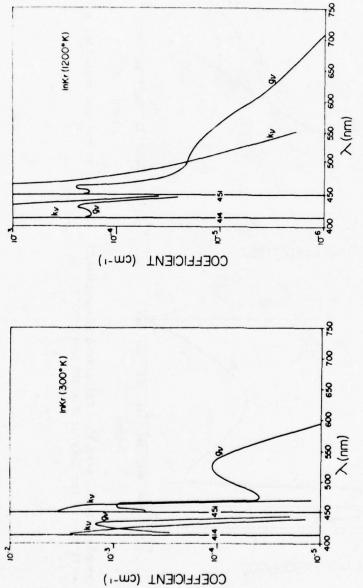


Graphical Data. A-12.12. Calculated dipole transition moments for III 1/2 - I 1/2, III 1/2 - I 3/2, and III 1/2 - II 1/2 transitions in GaKr.

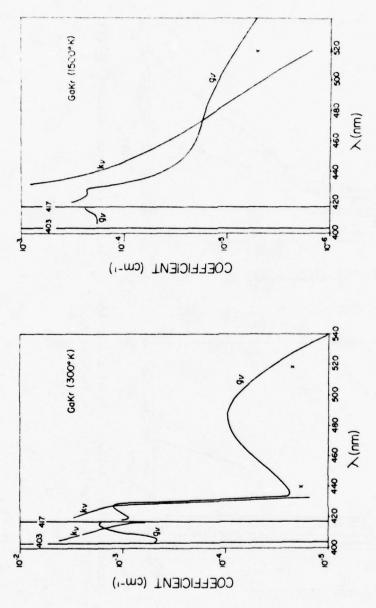
DIPOLE TRANSITION MOMENTS CONNECTING THE LOW-LYING STATES OF TIKE WITH SPIN-ORBIT CORRECTIONS



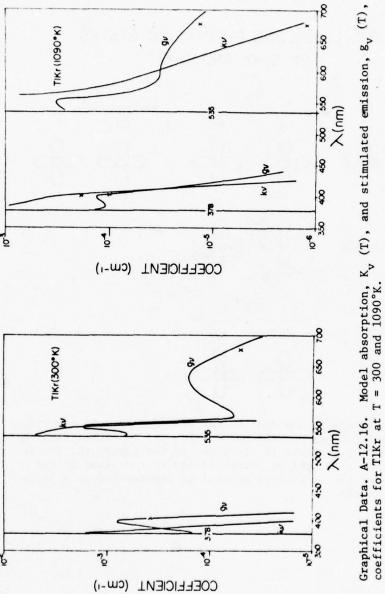
Graphical Data. A-12.13. Model dipole transition moments for the III 1/2 - I 1/2, III 1/2 - I 3/2, and III 1/2 - II 1/2 transitions in TlKr.



Graphical Data. A-12.14. Model absorption, K $_{\rm V}$ (T), and simulated emission, $\rm g_{\rm V}$ (T), coefficients for InKr at T = 3000 and 1200°K.



Graphical Data. A-12.15. Calculated absorption, K $_{\rm V}$ (T), and stimulated emission, $_{\rm R}$ (T), coefficients for GaKr at T = 300 and 1500 $^{\circ}$ K.



THE LOW-LYING ELECTRONIC STATES OF GaKr AND GaKr *

	2	Σ+	2	П
VALENCE	Go H	Kr C	Go	κ,
	9	9	T	9
RYDBERG	(gb)	A)		
	Go+	Kr Kr		
ION	offe	afo		

Graphical Data. A-12.17. Orbital diagrams for the low-lying electronic states of GaKr and GaKr⁺. The two lobed figures represent 4p orbitals in the plane of the paper; the circle represents a 4p orbital perpendicular to the plane of the paper; and the 5s Rydberg orbital is represented by a large dashed circle.

A-13. POTENTIAL ENERGY CURVES AND SPECTROSCOPIC CONSTANTS FOR AuH, AuC ℓ , $\mathrm{HgC}\ell_2$, AND HgH

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A-13. References:

 P. J. Hay, W. R. Wadt, L. R. Kahn, and F. W. Bobrowicz, "Ab Initio Studies of AuH, AuCl, HgH and HgCl₂ Using Relativistic Core Potentials," J. Chem. Phys. 69, 984 (1978).

Tabular Data. A-13.1. Orbital energies (in hartree) and radial expectation values (in bohr) for Au and Hg from relativistic and nonrelativistic wavefunctions.

	Nonrelativistic Hartree-Fock	Relativistic Hartree-Fock ^a	Dirac- Hartree-Fockb-d
	C	orbital energies	ereally services
Au atom			
5d	-0.5210	-0.6047	-0.4547 (-0.4287(5d.
6 <i>s</i>	-0.2208	-0.2902	$\begin{array}{c} -0.4547 \\ -0.2917 \end{array} \begin{cases} -0.4287(5d_{\star}) \\ -0.4935(5d_{\star}) \end{cases}$
6p	-0.1182	-0.1264	•••
Hg atom			
5 <i>d</i>	-0.7141	-0.6047	-0.6048 (-0.5746(5d.)
6s	-0.2620	-0.3267	$\begin{array}{c} -0.6048 \left\{ -0.5746(5d_{\star}) \right. \\ -0.3280 \left\{ -0.6501(5d_{\star}) \right. \end{array}$
6 <i>p</i>	-0.1716	-0.1778	•••
Au atom		(r)	
5 <i>d</i>	1.54	1.58	1 59 (1.62(5d ₊)
6 <i>s</i>	3.70	3.07	$\begin{array}{c} 1.59 \\ 3.06 \end{array} \begin{cases} 1.62(5d_{\star}) \\ 1.54(5d_{\star}) \end{cases}$
6p	5.54	5.14	5.12
Hg atom			
5 <i>d</i>	1.43	1.47	$\begin{array}{c} 1.47 \\ 2.84 \end{array} \begin{cases} 1.50(5d_{\bullet}) \\ 1.43(5d_{\bullet}) \end{cases}$
68	3.33	2.84	2 84 (1.43(5d)
65	4.26	4.07	•••

 $^{^{\}mathrm{a}}\mathrm{present}$ work using Cowan-Griffin method, A-13 Ref. 1.

b Averaged over fine-structure components.

 $^{^{\}mathrm{c}}$ J. B. Mann (unpublished and calculations).

 $^{^{\}mathrm{d}}$ J. P. Desclaux, At. Data Nucl. Data Tables $\underline{12}$, 311 (1973).

Tabular Data. A-13.2. Comparison of excitation energies in (eV) for the lowest states of ${\tt Au}$ and ${\tt Hg}$ atoms from all-electron calculations.

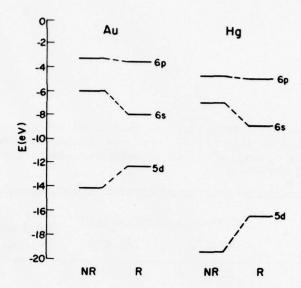
	Hartree- Fock	Relativistic Hartree- Fock ^a	Dirac- Hartree- Fock ^{b,d}	Exptl b, c
		Au atom		
5d ¹⁰ 6s ¹ (2S)	0.00	0.00	0.00	0.00
5d9 6s2 (2D)	5.13	1.86	1.86	1.74
5d ¹⁰ 6p ¹ (² P)	2.71	4.24	4.24	4.95
		Hg atom		
5d ¹⁰ 6s ² (¹ S)	0.00	0.00		0.00
5d ¹⁰ 6s 6p (³ P)	2,15	3.81		5.18
5d ¹⁰ 6s 6p (¹ P)	4.14	5.66		6.70

^aPresent work using Cowan-Griffin method, A-13 Ref. 1.

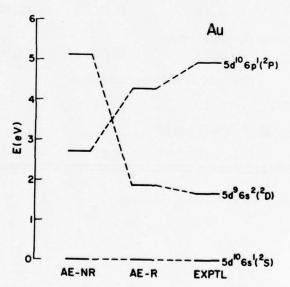
b Averaged over fine-structure components.

^CC. E. Moore, "Atomic Energy Levels," Natl. Bur. Stand. (U.S.) Circ. 476 (1958), Vol. III.

 $^{^{}m d}_{
m J.}$ B. Mann (unpublished calculations).



Graphical Data. A-13.3. Orbital energies of the valence electrons in Au and Hg atoms from nonrelativistic (NR) and relativistic (R) all-electron calculation. The 6p energies correspond to the $5d^{10}6p^1$ and $5d^{10}6p^1(^3P)$ configurations, respectively.



Graphical Data. A-13.4. Comparison of the energies of the lowest three states of Au atom from nonrelativistic (NR) all-electron calculations with experimental energies.

Tabular Data. A-13.5. Comparison of the excitation energies (in eV) for Hg atom computed from all-electron and valence-electron calculations, where the valence electron calculations explicitly treated the outer 12 electrons of Hg.

	Excitation energies (eV)		Ground state total energies	
	${}^{1}S \rightarrow {}^{3}P$	${}^{1}S \rightarrow {}^{1}P$	(hartree)	
Expt ^a	5.18	6.70		
	Relativistic o	alculations		
All-electron HF	3.81	5.66		
Valence-electron	(3s3p3d) basis			
HF	3.81	5.88	-43.47818	
MC-SCF	4.58	6.65	-43.50711	
Valence-electron	(3s4p4d) basis			
HF	3.78	5.64	-43.55284	
	Nonrelativistic	calculations		
All-electron HF	2.15	4.14		
Valence-electron	(3s3p4d) basis			
HF	2.04	4.21	-44.14543	

 $^{^2}$ Averaged over fine-structure components.

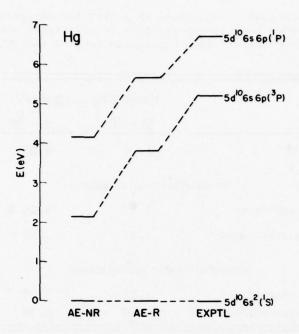
Tabular Data. A-13.6. Comparison of excitation energies for Au from all-electron and valence-electron calculations, where the valence-electron calculations explicitly treated the outer 11 electrons of Au.

	Excitation energy (eV	
	$^2S \leftarrow ^2D$	$^2S \leftarrow ^2P$
Expt ^a	1.74	4.95
Relativ	istic calculation	ns
All-electron	1.86	4.24
Valence-electron	1.67	4.22
Nonrelativ	ristic calculatio	ns
All-electron	5.13	2.71
Valence-electron	4.87	2.70

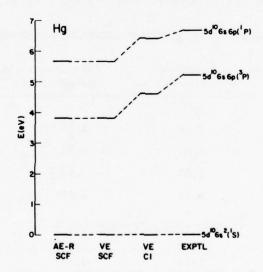
^aAveraged over fine-structure components.

Tabular Data. A-13.7. Comparison of excitation energies (in eV) for the states of the Au atom with spin-orbit coupling effects included.

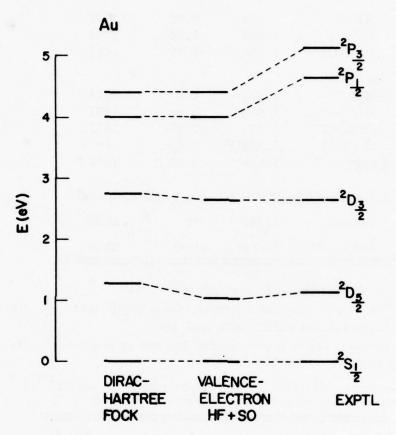
	Dirac- Hartree- Fock	Relativistic Hartree–Fock	Valence-electron Hartree-Fock	Expt
1S1/2	0.00	0.00	0.00	0.00
$^{2}D_{5/2}$	1.27	1.23	1.04	1.14
$^{2}D_{3/2}$	2.74	2.80	2.62	2,66
$^{2}P_{1/2}$	4.01	4.01	3.99	4.63
$^{2}P_{3/2}$	4.36	4.36	4.34	5,10
		Spin-orbit parame	eters (cm ⁻¹)	
5d	-4734	- 5105	(- 5105)	- 4910
6p	1879	1834	(1843)	2543



Graphical Data. A-13.8. Comparison of the energies of the lowest three states of Hg atom from nonrelativistic (NR) and relativistic (R) all-electron calculations with experimental energies.



Graphical Data. A-13.9 Comparison of relativistic all-electron (AE) and valence-electron (VE) results for the states of Hg atom where the relativistic ECP was used for the VE calculations.



Graphical Data. A-13.10. Comparison of valence-electron (VE) results for Au atom using the relativistic ECP and including spin-orbit coupling effects by perturbation theory with the results of Dirac-Hartree-Fock calculations and with experiment.

Tabular Data. A-13.11 Spectroscopic constants for $\mathrm{Au}^{197}\mathrm{H}$ computed from relativistic and nonrelativistic potentials.

$AuH-X^1\Sigma^+$	$R_e(\text{\AA})$	$D_e(eV)$	ω _e (cm ⁻¹
Nonrel. ECP			
HF	1.763	0.99	1387
GVB-1	1.820	1.52	1203
POL-CI	1.807	1.57	1217
Rel. ECP			
HF	1.508	1.55	2014
GVB-1	1.514	2.14	1891
POL-CI	1.522	2.23	1871
(1+2)CI	(1.5237)c	2.66	•••
Exptl ^a	1.5237	3.37	2305
1-Center num	erical Dirac	-Fock (all-	electron)b
Nonrel.	1.745		2296
Rel.	1.659 ^d	•••	2178

^aU. Ringstrom, Ark. Fys. <u>27</u>, 227 (1964).

Tabular Data. A-13.12. Spectroscopic constants for Au¹⁹⁷C1³⁷ from relativistic and nonrelativistic potentials.

AuCl— $X^1\Sigma^+$	$R_e(\text{\AA})$	$D_e(eV)$	$\omega_e(\text{cm}^{-1})$
Nonrel. ECP			
GVB-1	2.447	2.58	277
Rel. ECP			
GVB-1	2.283	1.96	298
POL-CI	2.291	2.39	306
Exptl ^{a, b}	• • •	3.5 ± 0.1	382

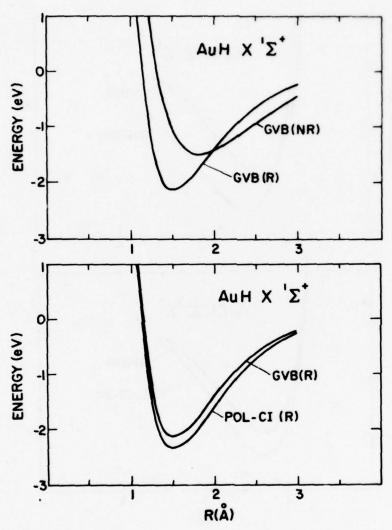
^aA. G. Gaydon, <u>Dissociation Energies</u> (Chapman and Hall, London, 1968).

bJ. P. Desclaux and P. Pyyko, Chem. Phys. Lett. 39, 300 (1976).

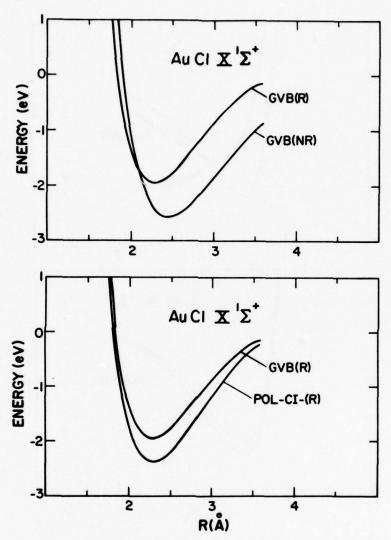
 $^{^{}m c}$ Experimental bond length assumed.

 $^{^{\}mathrm{d}}\mathrm{Using}$ a Morse potential fit instead of a quadratic fit leads to an R_e of 1.622 Å.

bB. Rosen, Spectroscopic Data (Pergamon, Oxford, 1970).



Graphical Data. A-13.13. (a) Potential energy curves for AuH using relativistic (R) and nonrelativistic (NR) potentials for GVB (2-configuration) wavefunctions. (b) Potentials energy curves for AuH using the R potentials with GVB and POL-CI wavefunctions.



Graphical Data. A-13.14. (a) Potential energy curves for AuCl using relativistic (R) and nonrelativistic (NR) potentials for GVB wavefunctions. (b) Potential energy curves for AuCl using the R potential with GVB and POL-CI wavefunctions.

Tabular Data. A-13.15. Calculated and experimental bond lengths and dissociation energies (into Hg + 2Cl) for ${\rm HgCl}_2.$

	R.(Å)		De(kcal/mole)	
	HF	2-config.	HF	2-config.
Rel. ECP	2,290	2,301	57.5	59.6
Nonrel, ECP	2.409	2,412	97.6	100.0
Nonrel. ECPe	2.313	2,315	:	115.7
Expt.	2.29±0.024, 2.252d		106.4b	

^ap.A. Akisin, V.P. Spiridonov, and A.N. Khodchenkov, Zh. Fiz.Khim. 33, 20 (1959); earlier determinations were discussed by L. R. Maxwell and V. M. Mosley, Phys. Rev. 57, 21 (1940).

bJANAF Thermochemical Tables" Natl. Stand. Ref. Data Ser. Natl. Bur. Stand. 37 (1971) where zero-point corrections have not been applied.

CH. Basch, M.D. Newton, J. Jafri, J.W. Moskowitz and S. Topiol, J. Chem. Phys. (in press).

d_{K.} Kashiwabara, S. Konaka, and M. Kimura, Bull. Chem. Soc. Jpn <u>46</u>, 410 (1973)

Tabular Data. A-13.16. Ionization potentials (in eV) for ${\rm HgCl}_2$ from orbital energies (- ϵ_i) and from separate SCF calculations (ΔE - SCF).

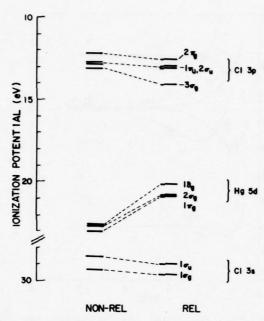
	$-\epsilon_i$ (Nonrel.)	$-\epsilon_i$ (Rel.)	Δ E-SCF (Rel.)	Exptl ^a
2π _g (3p _{C1})	12.21	12.56	11.98	11.43
$1\pi_u (3p_{C1})$	12.64	13.06	12.48	12.13
$2\sigma_{u} (3p_{C1})$	12.86	13.01	12.43	12.74
$3\sigma_g (3p_{C1})$	13.08	14.09	13.60	13,74
$1\delta_g \ (5d_{\mathrm{H}g})$	22.66	20.14	17.15	
$1\pi_{\rm g}$ $(5d_{\rm Hg})$	22.99	20.81	17.98	
$2\sigma_{\rm g}~(5d_{\rm Hg})$	22.67	20.70	18.63	
$1\sigma_{\!\scriptscriptstyle u} \ (3s_{\rm Cl})$	28.58	29.00		
1σ _ε (3s _{C1})	29.35	29.62		

 $^{^{}a}$ J.H.D. Elana, Int. J. Mass. Spectrom. Ion Phys. $\underline{4}$, 37 (1970).

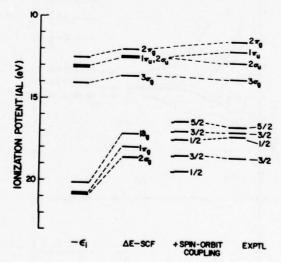
Tabular Data. A-13.17. Calculated and experimental ionization potentials for the 5d orbitals of ${\rm HgCl}_2$, where spin-orbit coupling effects have been included.

State (Ω)	$-\epsilon_i$ with $S-O$ coupling	ΔE -SCF with S - O coupling	Exptl ^a
5/2	19.39	16.40	16.71
3/2	19.88	16.99	17.05
1/2	20.00	17.51	17.27
3/2	21.44	18.51	18,65
1/2	21.89	19.42	•••

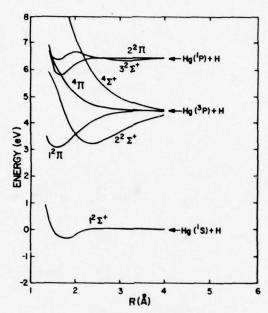
 $^{^{}a}$ J.H.D. Elana, Int. J. Mass. Spectrom. Ion Phys. $\underline{4}$, 37 (1970).



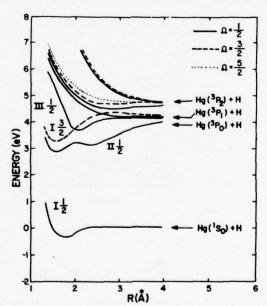
Graphical Data. A-13.18. Orbital energies of ${\rm HgC}\ell_2$ from Hartree-Fock calculations using relativistic and nonrelativistic potentials for Hg.



Graphical Data. A-13.19. Ionization potentials for $\mathrm{HgC}\ell_2$ using the relativistic potential for Hg as predicted from Koopmans' theorem (- ϵ_i) and from separate SCF calculations ($\Delta \mathrm{E-SCF}$).



Graphical Data. A-13.20. Potential energy curves for the lowest states of HgH without spin-orbit coupling effects.



Graphical Data. A-13.21. Potential energy curves for the lowest states of HgH including spin-orbit coupling effects. The states dissociating to ${\rm Hg(}^1{\rm P)}$ + H are not shown.

Tabular Data. A-13.22. Spectroscopic constants for the states of $^{\rm 202}{\rm HgH}.$

	$R_e(\text{\AA})$	$D_e(eV)$	$\omega_e(\mathrm{cm}^{-1})$	$T_e(eV)$			
	States without	spin-orbit	coupling				
X ² Σ*							
Present	1.763	0.33	1227	0.00			
Das, Wahla	1.783	0.37	1123	0.00			
Exptl ^{b,c}	1.7404	0.46	1387	0.00			
1 ² Π							
Present	1.574	1.41	1693	3,32			
Das, Wahl	1.593	•••	2032	3.80			
2 ² Σ*							
Present	2.390	1.25		3.46			
Das, Wahl							
St	ates including	spin-orbit	coupling				
$\Pi_{\frac{1}{2}}(^2\Pi_{1/2})$							
Present	1.579	1.09	1629	3,11			
Exptl	1.586	2.08	2066	3.05			
$I^{\frac{3}{2}}(^2\Pi_{3/2})$							
Present	1.575	0.98	1686	3.48			
Exptl	1.580	1.85	2067	3.50			
III $\frac{1}{2}$ (2 $^2\Sigma_{1/2}^+$)							
Present	2.078	0.53	1604	3.94			
Exptl	$(r_0 = 2.03)$	1.15	•••	4.20			

^aG. Das and A. C. Wahl, J. Chem. Phys. <u>64</u>, 4672 (1974).

^bT. L. Porter, J. Opt. Soc. Am. <u>52</u>, 1201 (1962).

cW. C. Stwalley, J. Chem Phys. <u>63</u>, 3062 (1975).

A-14. POTENTIAL ENERGY CURVES, ELECTRONIC ENERGIES, AND SPECTROSCOPIC CONSTANTS FOR VALENCE STATES OF $\mathbf{0}_2$

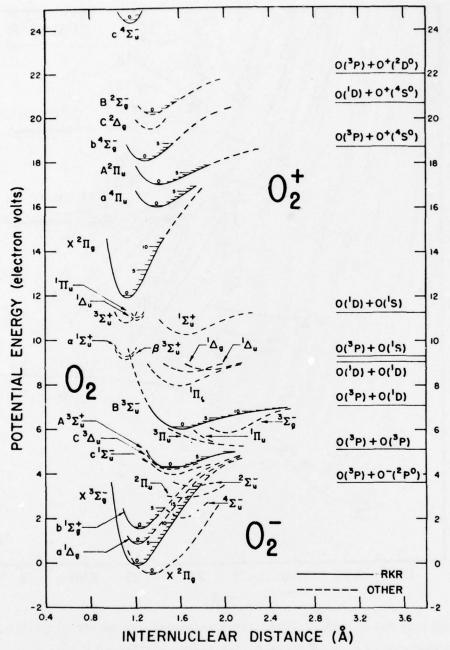
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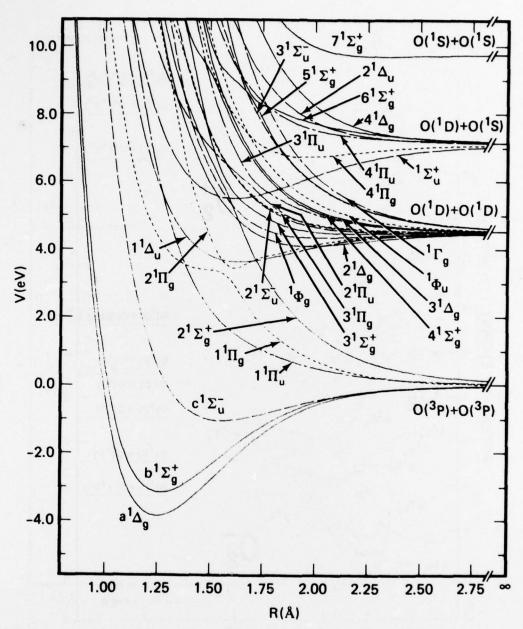
A-14. References:

- R. P. Saxon and B. Liu, "Ab initio Configuration Study of the Valence States of O₂," J. Chem. Phys. 67, 5432 (1977).
- 2. P. Krupenie, "The Spectrum of Molecular Oxygen," J. Phys. Chem. Ref. Data. 1, 423 (1977)*.
- H. F. Schaefer and F. E. Harris, "Ab initio Calculations on 62 Low-Lying States of the 0₂ Molecule," J. Chem. Phys. 48, 4946 (1968).
- 4. B. J. Moss and W. A. Goddard, "Configuration Interaction Studies on Low-Lying States of 0_2^* ," J. Chem. Phys. <u>63</u>, 3523 (1975).

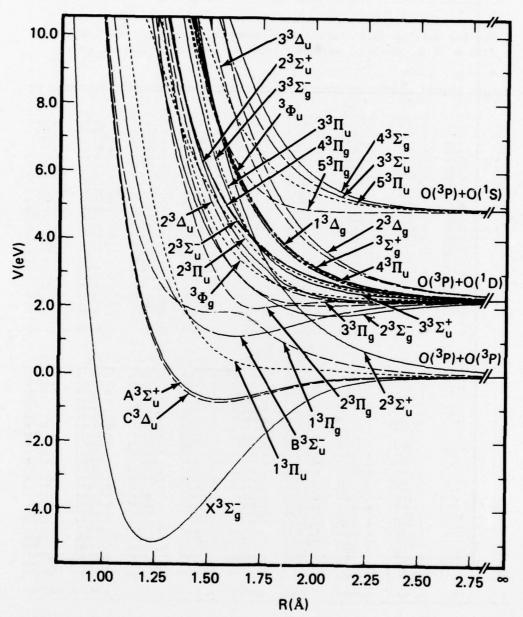
Reference 2 is a critical review and compilation of the observed and predicted spectroscopic data on 0_2 and its ions 0_2^- , 0_2^+ , and 0_2^{2+} . The ultraviolet, visible, infrared, Raman, microwave, and electron para-magnetic resonance spectra are included. Each electronic band system is discussed in detail, and tables of band origins and heads are given. The microwave and EPR data are also tabulated. Special subjects such as the dissociation energy of 0_2 , perturbations, and predissociations are discussed. Potential energy curves are given, as well as f-values, Franck-Condon integrals, and other intensity factors. A summary table lists the molecular constants for all known electronic states of 0_2 and 0_2^+ . Electronic structure and theoretical calculations are also discussed.



Graphical Data. A-14.1. Potential energy curves for 0_2^- , 0_2^- , and 0_2^+ .



Graphical Data. A-14.2. Calculated potential curves for singlet valence states of 0_2 . Energies are given relative to $0 \, (^3P) + 0 \, (^3P)$.



Graphical Data. A-14.3. Calculated potential curves for triplet valence states of 0_2 . Energies are given relative to $0\ (^3P)$ + $0\ (^3P)$.

Tabular Data. A-14.4 Calculated potential curves for 62 valence states of $\boldsymbol{0}_2$ given in hartrees relative to the asymptotic energy of each state.

							-		
R(a ₀)	$b^1\Sigma_g^+$	21 E	$3^1\Sigma_g^+$	41 E	$5^1\Sigma_q^+$	$6^1\Sigma_q^+$	715 ·	15.	C1Σ
1.8	0.10650	0.62422	0.81921	0. 93779	0.87063	0.91214	0.87560	0.48987	0.48807
2.0	-0.04505	0.51873	C.54599	0.63957	0.65576	0.59581	0.64727	0. 24 190	0.22479
2.2	-0.10362	0.49603	0.37025	0.41849	0.57767	C.51852	0.43434	0.09649	0.08365
2.3	-0.11384	0.46416	C.33526	0.35037	0.49961	0.46287	0.39552	0.04919	0.04091
2.4	-0.11043	0.40 122	0.30070	0.34183	C.39506	0.38980	0.35502	0.01368	0.01068
2.6	-0.16791	0.31138	0.22689	0.23073	0.32221	C. 27880	0.29188	-0.03164	-0.02397
2.8	-0.09069	0.25123	C.11568	0.17928	0.21730	0. 22615	0.21178	-0.05347	-0.03717
3.0	-0.07133	0.20055	0.04904	0.12488	0.16833	0.11892	0.15911	-0.06056	-0.03879
3. 2	-0.05327	0.14393	C. C2474	0.03006	0.14368	0.05140	0.08909	-0.05882	-0.03472
3.4	-0.03317	0.10261	0.01038	0.05043	C. C 9958	C.03626	0.04508	-0.05231	-0.02850
3.5	-0.C319C	0.03646	0.00581	0.03997	0.08297	C.03116	0.03040	-0.04816	-0.02524
3.6	-0.02649	0.07276	0.00256	0.03170	0.06931	0.02688	0.01949	-0.04375	-0.02209
3.8	-0.01831	0.05138	-0.00105	0.01998	0.04864	C.02006	0.00607	-0.03493	-0.01649
4.0	-0.01214	0.03619	-0.C0220	0.01264	0.03427	0.01493	-0.00009	-0.02694	-0.01203
4.5	-0.00453	0.01499	-0.00148	0.00400	0.01436	0.00702	-0.00272	-0.01303	-0.00534
5.0	-0.00189	0.00624	-C.CCC50	0.00115	0.00612	0.00333	-0.00151	-0.00623	-0.00244
5.5	-0.00093	0.00265	-0.00009	0.00020	0.00272	0.00166	-0.00068	-0.00316	-0.00119
6.0	-0.00339	0.00117	C.CCCO4	-0.00011	0.00129	0.00089	-0.00033	-0.00175	-0.00062
6.5	-0.00119	0.00054	C.00005	-0.00016	0.00067	0.00051	-0.00018	-0.00105	-0.00036
7.0	-0.00010	0.00027	0.00003	-0.00C12	0.00C37	C.00032	-0.00011	-0.00067	-0.00021
7.5	-0.00005	0.00015	C.0CC02	-0.00008	0.00022	0.00022	-0.00007	-0.00045	-0.00013
8.0	-0.00002	0.00009	0.00002	-0.00005	0.00014	0.00016	-0.00005	-0.00031	-0.00008
9.0	0.00000	0.00004	0.00002	-0.00002	U.CCC07	0.00009	-0.00002	-0.00016	-0.00004
10.0	0.00001	0.00003	C.COCC2	-0.00001	0.00004	0.00006	-0.00001	-0.00009	-0.00001
20.0	0.00000	0.00125	6. 16571	0.16600	0.16625	0.26219	0.35923	0.26219	-0.00000
R(a ₀)	2¹ Σ.	3 ¹ Σ ₀ -	1 ¹ П _а	21110	3 ¹ 11 ₀	4 ¹ П _а	1 ¹ П _и	2111,	3¹ II.
				2 ¹ [1 _g	3 ¹ 11 _g	4 ¹ П _g			
1.8	0.59036	0.72444	0.50684	0.38172	0.39743	0.76760	0.70054	0.57396	0.59596
1.8	0.59036	0.72444	0.50684	0.38172	0.39743 0.29786	0.76760 0.57251	0.70054 0.50662	0.57396	0.59596 0.48550
1.8 2.0 2.2	0.59036 0.48587 0.45371	0.72444 0.65267 C.49053	0.50684 0.32532 C.20859	0.38172 0.24879 0.23629	0.39743 0.29786 0.28489	0.76760 0.57251 0.30248	0.70054 0.50662 0.33331	0.57396 0.38767 0.26014	0.59596 0.48550 0.46368
1.8 2.0 2.2 2.3	0.59036 0.48587 0.45371 0.38626	0.72444 0.65267 C.49053 0.45984	0.50684 0.32532 C.2C859 0.17509	0.38172 0.24879 0.23629 0.24471	0.39743 0.29786 0.28489 0.29205	0.76760 0.57251 0.30248 C.19934	0.70054 0.50662 0.33331 0.26410	0.57396 0.38767 0.26014 0.21669	0.59596 0.48550 0.46368 0.43307
1.8 2.0 2.2 2.3 2.4	0.59036 0.48587 0.45371 0.38626 0.30725	0.72444 0.65267 C.49053 0.45984 C.46294	0.50684 0.32532 C.2C859 0.17509 C.15253	0.38172 0.24879 0.23629 0.24471 0.20847	0.39743 0.29786 0.28489 0.29205 0.25949	0.76760 0.57251 0.30248 C.19934 0.20914	0.70054 0.50662 0.33331 0.26410 0.20858	0.57396 0.38767 0.26014 0.21669 0.18150	0.59596 0.48550 0.46368 0.43307 0.39737
1.8 2.0 2.2 2.3 2.4 2.6	0.59036 0.48587 0.45371 0.38626 0.30725 0.19072	0.72444 0.65267 C.49053 0.45984 C.46294 0.42491	0.50684 0.32532 C.20859 0.17509 C.15253 0.12935	0.38172 0.24879 0.23629 0.24471 0.20847 0.08402	0.39743 0.29786 0.28489 0.29205 0.25949 0.18976	0.76760 0.57251 0.30248 C.19934 0.20914 C.18861	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135	0.57396 0.38767 0.26014 0.21669 0.18150 0.12955	0.59596 0.48550 0.46368 0.43307 0.39737 0.28989
1.8 2.0 2.2 2.3 2.4 2.6 2.8	0.59036 0.48587 0.45371 0.38626 0.30725 0.19072 0.11579	0.72444 0.65267 C.49053 0.45984 C.46294 0.42491 0.29095	0.50684 0.32532 C.20859 0.17509 C.15253 0.12935 C.12353	0.38172 0.24879 0.23629 0.24471 0.20847 0.08402 0.00285	0.39743 C.29786 O.28489 C.29205 O.25949 O.18976 O.11464	0.76760 0.57251 0.30248 0.19934 0.20914 0.18861 0.09548	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135	0.57396 0.38767 0.26014 0.21669 0.18150 0.12955 0.09470	0.59596 0.48550 0.46368 0.43307 0.39737 0.28989 0.17539
1.8 2.0 2.2 2.3 2.4 2.6 2.8 3.0	0.59036 0.48587 0.45371 0.38626 0.30725 0.19072 0.11579 0.06823	0.72444 0.65267 C.49053 0.45984 C.46294 0.42491 0.29095 0.20045	0.50684 0.32532 0.20859 0.17509 0.15253 0.12935 0.12353 0.11408	0.38172 0.24879 0.23629 0.24471 0.20847 0.08402 0.00285	0.39743 0.29786 0.28489 0.29205 0.25949 0.18976 0.11464 0.06808	0.76760 0.57251 0.30248 C.19934 0.20914 C.18861 0.09548 0.03756	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135 0.08581 0.05909	0.57396 0.38767 0.26014 0.21669 0.18150 0.12955 0.09470 0.06970	0.59596 0.48550 0.46368 0.43307 0.39737 0.28989 0.17539 0.10133
1.8 2.0 2.2 2.3 2.4 2.6 2.8 3.0 3.2	0.59036 0.48587 0.45371 0.38626 0.30725 0.19072 0.11579 0.06323 0.03845	0.72444 0.65267 C.49053 0.45984 C.46294 0.42491 0.29095 0.20045 0.13924	0.50684 0.32532 C.20859 0.17509 C.15253 0.12935 C.12353 0.11408 C.C7824	0.38172 0.24879 0.23629 0.24471 0.20847 0.08402 0.0285 -0.03843 -0.03235	0.39743 0.29786 0.2489 0.29205 0.25949 0.18976 0.11464 0.06808 0.03941	0.76760 0.57251 0.30248 C.19934 0.20914 C.18861 0.09548 0.03756 0.00523	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135 0.08581 0.05909 0.04264	0.57396 0.38767 0.26014 0.21669 0.18150 0.1295 0.09470 0.06970 0.04853	0.59596 0.48550 0.46368 0.43307 0.39737 0.28989 0.17539 0.10133 0.05753
1.8 2.0 2.2 2.3 2.4 2.6 2.8 3.0 3.2 3.4	0.59C16 0.485d7 0.45371 0.38626 0.30725 0.19072 0.11579 0.06323 0.03845	0.72444 0.65267 C.49053 0.45984 C.46294 0.42491 0.29095 0.20045 0.13924 0.09742	0.50684 0.32532 C.20859 0.17509 C.15253 0.12935 C.12353 0.11408 C.C7824 0.05342	0.38172 0.24879 0.23629 0.24471 0.20847 0.08402 0.00285 -0.03843 -0.03235 -0.02529	0.39743 C.29786 0.24489 C.29205 0.18976 0.11464 C.06808 0.03941 0.02215	0.76760 0.57251 0.30248 C.19934 0.20914 C.18861 0.09548 0.03756 0.00523 -C.01011	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135 0.08581 0.05909 0.04264 0.03145	0.57396 0.38767 0.26014 0.21669 0.18150 0.12955 0.09470 0.06970 0.04853 0.02660	0.59596 0.48550 0.46368 0.43307 0.39737 0.28989 0.17539 0.10133 0.05753 0.03780
1.8 2.0 2.2 2.3 2.4 2.6 2.8 3.0 3.2 3.4 3.5	0.59036 0.485371 0.45371 0.38626 0.30725 0.19072 0.11579 0.06423 0.03845 0.02329 0.01425	0.72444 0.65267 C.49053 0.45984 C.46294 0.29095 0.29095 0.13924 0.09742 0.08166	0.50684 0.32532 C.20859 0.17509 C.15253 0.12935 C.12353 0.11408 C.C7822 0.05342 0.05342	0.38172 0.24879 0.23629 0.24471 0.20847 0.08402 0.00285 -0.03843 -0.03235 -0.02529 -0.02194	0.39743 C.29786 0.28489 C.29205 0.25949 0.18976 0.11464 C.06808 0.03941 0.02215 0.01646	0.76760 0.57251 0.30248 C.19934 0.20914 C.18861 0.09548 0.03756 0.00523 -C.01011	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135 0.08581 0.05909 0.04264 0.03145 0.02703	0.57396 0.38767 0.26014 0.21669 0.18150 0.12955 0.09470 0.06970 0.04853 0.02660 0.01865	0.59596 0.48550 0.46368 0.43307 0.39737 0.28989 0.17539 0.10133 0.05753 0.03780 0.03128
1.8 2.0 2.2 2.3 2.4 2.6 2.8 3.0 3.2 3.4 3.5 3.6	0.59C36 0.485d7 0.485d7 0.45371 0.38626 0.30725 0.19072 0.11579 0.06423 0.03845 0.02329 0.01425 0.00471	0.72444 0.65267 C.49053 0.45984 C.46294 0.42491 0.29095 0.20045 0.13924 0.09742 0.08166 0.06852	0.50684 0.32532 C.2C859 0.17509 C.15253 0.12935 C.12353 0.11408 C.C7824 0.05342 0.04401	0.38172 0.24879 0.23629 0.24471 0.20847 0.04402 0.00285 -0.03843 -0.03235 -0.02529 -0.02194 -0.01885	0.39743 0.29786 0.28489 0.29205 0.25949 0.18976 0.11464 0.06808 0.03941 0.02215 0.01646 0.01220	0.76760 0.57251 0.30248 C.19934 0.20914 C.18861 0.09548 0.03756 0.00523 -C.01011 -0.01364 -0.C1533	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135 0.08581 0.05909 0.04264 9.03145 0.02703 0.02317	0.57396 0.38767 0.26014 0.21669 0.18150 0.12955 0.09470 0.06970 0.04853 0.02660 0.01865 0.01287	0.59596 0.48550 0.46368 0.43307 0.39737 0.28989 0.17539 0.10133 0.05753 0.03780 0.03128 0.02581
1.8 2.0 2.2 2.3 2.4 2.6 2.8 3.0 3.2 3.4 3.5 3.6 3.8	0.59C36 0.48537 0.45371 0.38526 0.30725 0.19072 0.11579 0.06423 0.03845 0.02029 0.01425 0.00471 0.00471	0.72444 0.65267 C.49053 0.45984 0.42491 0.29095 0.20045 0.13924 0.08166 0.06852 0.04834	0.50684 0.32532 C.20859 0.17509 0.175253 0.12353 0.11408 C.C7824 0.05342 0.04401 0.03616 C.C241b	0.38172 0.24879 0.23629 0.24471 0.20847 0.08402 0.00285 -0.03843 -0.03235 -0.02529 -0.02194 -0.01885 -0.01355	0.39743 0.25786 0.24489 0.29205 0.25949 0.18976 0.11464 0.06808 0.03941 0.02215 0.01646 0.01220	0.76760 0.57251 0.30248 C.19934 C.18861 0.09548 0.03756 0.00523 - C.01011 -0.01364 -0.01533	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135 0.08581 0.05909 0.04264 0.03145 0.02703 0.02317 0.01684	0.57396 0.38767 0.26014 0.21669 0.18150 0.12955 0.09470 0.04853 0.02660 0.01865 0.01287 0.00598	0.59596 0.48550 0.46368 0.43307 0.39737 0.28989 0.17539 0.10133 0.05753 0.03780 0.03128 0.02561 0.01735
1.8 2.0 2.2 2.3 2.4 2.6 2.8 3.0 3.2 3.4 3.5 3.6 3.6	0.59C16 0.485d7 0.45371 0.38626 0.30725 0.19072 0.11579 0.06423 0.03845 0.02J29 0.01425 0.00471 0.00394 0.00104	0.72444 0.65267 C.49053 0.45984 C.46294 0.29095 0.20045 0.13924 0.09742 0.08166 0.06852 0.04834 0.03414	0.50684 0.32532 C.20859 0.17509 C.15253 0.12935 C.12353 0.11408 C.07824 0.054401 0.03616 C.0241b	0.38172 0.24879 0.23629 0.24471 0.20847 0.04402 0.00285 -0.03235 -0.03235 -0.02529 -0.01885 -0.01355 -0.01355	0.39743 0.29786 0.24489 0.29905 0.25949 0.18976 0.11464 0.06808 0.03941 0.02215 0.01646 0.01220 0.00674 0.00380	0.76760 0.57251 0.30248 0.20914 0.20914 0.09548 0.03756 0.00523 -C.01011 -0.01364 -0.01523 -0.01526	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135 0.08581 0.05909 0.04264 0.03145 0.02703 0.02317 0.01684 0.01203	0.57396 0.38767 0.26014 0.21669 0.18150 0.12955 0.09470 0.06970 0.04853 0.02660 0.01865 0.01287 0.00598	0.59596 0.48550 0.46368 0.43307 0.39737 0.28989 0.17539 0.10133 0.05753 0.03780 0.03128 0.02581 0.01735
1.8 2.0 2.2 2.3 2.4 2.6 2.8 3.0 3.2 3.4 3.5 3.6 4.0	0.59C16 0.485d7 0.453d7 0.38026 0.30725 0.19072 0.06423 0.03845 0.02029 0.01425 0.00704 0.00104 0.00104	0.72444 0.65267 C.49053 0.45984 C.46294 0.42491 0.29095 0.13924 0.09742 0.08166 0.06852 0.04834 0.03414	0.50684 0.32532 C.20859 0.17509 C.15253 0.11408 C.C7824 0.05342 0.03616 C.C241b 0.01590 0.00495	0.38172 0.24879 0.23629 0.24471 0.20847 0.08402 0.0285 -0.03843 -0.03235 -0.02529 -0.02194 -0.01365 -0.03949 -0.00378	0.39743 0.29786 0.28489 0.29205 0.25949 0.18976 0.11464 0.06808 0.03941 0.02215 0.016406 0.01220 0.00674 0.00390 0.00091	0.76760 0.57251 0.30248 0.19934 0.20914 0.03756 0.00523 -C.01011 -0.01364 -0.01533 -0.01526 -0.01529	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135 0.09581 0.05909 0.04264 2.03145 0.02703 0.02317 0.01684 0.01203	0.57396 0.38767 0.26014 0.21669 0.18150 0.12955 0.09470 0.06970 0.04853 0.02660 0.01287 0.00598 0.00281	0.59596 0.48550 0.46368 0.43307 0.39737 0.28989 0.17539 0.10133 0.05753 0.03128 0.02581 0.02581 0.01735 0.01148
1.8 2.0 2.2 2.3 2.4 2.8 3.0 3.2 3.4 3.5 3.6 4.5	0.59C36 0.483d7 0.45371 0.38026 0.30725 0.19072 0.06423 0.03845 0.02229 0.01425 0.00471 0.00104 -0.00089	0.72444 0.65267 C.49053 0.45984 C.46294 0.29095 0.29095 0.20045 0.09742 0.09742 0.0852 0.04854 0.03414 0.01431	0.50684 0.32532 C.20859 0.17509 C.15253 0.12935 0.11408 C.C7824 0.05342 0.05342 0.05342 0.05495 0.00495 0.00495 0.00495	0.38172 0.24879 0.23629 0.24471 0.08402 0.003402 0.00285 -0.03843 -0.03235 -0.02529 -0.02194 -0.01865 -0.01375 -0.00378	0.39743 C.29786 0.24489 C.29205 0.25949 0.18976 0.11464 C.06808 0.03941 0.02215 0.01646 0.01220 0.00674 0.00380 0.00091	0.76760 0.57251 0.30248 0.19934 0.20914 0.09548 0.03756 0.00523 -0.01011 -0.01364 -0.01533 -0.01526 -0.01298 -0.00688	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135 0.08581 0.05909 0.04264 0.03145 0.02317 0.02317 0.01684 0.01203 0.00475 0.00162	0.57396 0.38767 0.26014 0.21669 0.18150 0.12955 0.09470 0.06970 0.04853 0.02660 0.01287 0.00598 0.00281 0.00008	0.59596 0.48550 0.46368 0.43307 0.39737 0.17539 0.17539 0.03780 0.03780 0.03128 0.01735 0.01148 0.00381
1.8 2.0 2.2 2.3 2.4 2.8 3.0 3.2 3.5 3.6 3.6 4.0 5.5	0.59C16 0.485d7 0.45371 0.38626 0.30725 0.19072 0.11579 0.06423 0.03245 0.02129 0.01425 0.00471 0.00394 0.00004 0.00084 0.00084	0.72444 0.65267 C.49053 0.45984 C.46294 0.29095 0.20045 0.13924 0.09742 0.08166 0.06852 0.04834 0.03414 0.01431 0.00607 0.00607	0.50684 0.32532 C.20859 0.17509 C.15253 0.12935 C.12353 0.11408 C.07824 0.03616 C.02416 0.01590 0.00495 0.00190	0.38172 0.24879 0.23629 0.24471 0.20847 0.08402 0.0285 -0.03235 -0.02529 -0.01355 -0.03649 -0.03649 -0.00376 -0.00376	0.39743 C.29786 O.24489 C.29205 O.25949 O.18976 O.11464 C.06808 O.03941 O.02215 O.01646 O.01220 O.00674 O.00010	0.76760 0.57251 0.30248 0.19934 0.20914 0.09548 0.03756 0.00523 - C.01011 -0.01364 -0.01523 -0.01526 -0.01298 -0.00325 -0.00325	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135 0.08581 0.05909 0.04264 0.0270 0.02317 0.01684 0.01203 0.0475 0.00475	0.57396 0.38767 0.26014 0.21669 0.18150 0.12955 0.09470 0.06970 0.04853 0.02660 0.01865 0.01287 0.00598 0.00281 0.00008	0.59596 0.48550 0.46368 0.43307 0.39737 0.10133 0.05753 0.03780 0.03128 0.01735 0.01735 0.01148 0.00381 0.00107
1.8 2.0 2.2 2.3 2.4 2.6 2.8 3.0 3.2 3.4 3.5 3.6 4.5 5.0 5.0	0.59C16 0.485d7 0.45371 0.38026 0.30725 0.11579 0.06423 0.03845 0.02129 0.01425 0.00104 0.00104 0.00064 0.00064	0.72444 0.65267 C.495984 C.46294 0.42491 0.29095 0.20045 0.13924 0.09742 0.08166 0.06852 0.04834 0.01431 0.01431 0.00607 0.00267	0.50684 0.32532 C.20859 0.17509 C.15253 0.12935 0.11408 C.07824 0.03416 0.03616 C.0241b 0.01590 0.00495 0.00495 0.00524	0.38172 0.24879 0.23629 0.24471 0.20847 0.09402 0.00285 -0.03843 -0.03235 -0.02529 -0.01885 -0.01355 -0.00949 -0.00165 -0.00066	0.39743 0.29786 0.28489 0.29205 0.25949 0.18976 0.11464 0.06808 0.03941 0.02215 0.01646 0.01220 0.00674 0.00380 0.00091 0.00011	0.76760 0.57251 0.30248 0.19934 0.20914 0.03756 0.00523 -C.01011 -0.01563 -0.01533 -0.01526 -0.01298 -0.00668 -0.00325 -0.00173	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135 0.08581 0.02703 0.02703 0.02317 0.01684 0.01203 0.00475 0.00162 0.00040	0.57396 0.38767 0.26014 0.21669 0.18150 0.0970 0.04853 0.02660 0.01885 0.01287 0.00598 0.00281 0.00281 0.00007	0.59596 0.48550 0.46368 0.43307 0.39737 0.17539 0.10133 0.05753 0.03780 0.02581 0.02581 0.01188 0.00381 0.00107 0.00015
1.8 2.0 2.2 2.3 2.6 2.8 3.0 3.2 3.4 3.5 3.6 3.8 4.0 5.0 5.5 6.0	0.59C36 0.483d7 0.45371 0.38026 0.30725 0.11579 0.06423 0.03845 0.02129 0.01425 0.00971 0.00104 -0.00089 -0.00084 -0.00064 -0.00046	0.72444 0.65267 C.49053 0.45984 C.46294 0.29095 0.20045 0.09742 0.09742 0.0852 0.04854 0.04834 0.03414 0.00607 0.00607 0.00607 0.00125	0.50684 0.32532 C.20859 0.17509 C.15253 0.12935 0.11408 C.07824 0.05342 0.05342 0.05490 0.00495 0.00495 0.00495 0.00495 0.00495 0.00495	0.38172 0.24879 0.23629 0.24471 0.08402 0.00285 -0.03285 -0.02529 -0.02194 -0.01865 -0.00378 -0.00378 -0.000378 -0.00052 -0.00065 -0.00086	0.39743 C.29786 0.24489 C.29205 0.25949 0.18976 0.03941 0.02215 0.01646 0.01220 0.00674 0.00380 0.00091 0.00010	0. 76760 0. 57251 0. 30248 0. 19934 0. 20914 0. 03756 0. 03756 0. 00523 -0. 01011 -0. 01364 -0. 01533 -0. 01526 -0. 01298 -0. 00068 -0. 00072 -0. 00172 -0. 00172 -0. 00172	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135 0.08581 0.05909 0.04264 0.03145 0.02317 0.01684 0.01203 0.00475 0.00000	0.57396 0.38767 0.26014 0.21669 0.18150 0.12955 0.09470 0.06970 0.04853 0.02660 0.01287 0.00598 0.00281 0.00008 -0.00008 -0.00008	0.59596 0.48550 0.46368 0.43307 0.39737 0.17539 0.10133 0.05753 0.03780 0.03128 0.02581 0.01735 0.01148 0.00381 0.00107 0.00015 -0.00013
1.8 2.0 2.2 2.3 2.4 2.6 2.8 3.0 3.5 3.6 3.6 4.0 4.5 5.5 6.0 5.5	0.59C16 0.485d7 0.45371 0.38026 0.30725 0.11579 0.06423 0.03845 0.02129 0.01425 0.00104 0.00104 0.00064 0.00064	0.72444 0.65267 C.495984 C.46294 0.42491 0.29095 0.20045 0.13924 0.09742 0.08166 0.06852 0.04834 0.01431 0.01431 0.00607 0.00267	0.50684 0.32532 C.20859 0.17509 C.15253 0.12935 0.11408 C.07824 0.03416 0.03616 C.0241b 0.01590 0.00495 0.00495 0.00524	0.38172 0.24879 0.23629 0.24471 0.20847 0.09402 0.00285 -0.03843 -0.03235 -0.02529 -0.01885 -0.01355 -0.00949 -0.00165 -0.00066	0.39743 C.25746 O.24489 C.25949 O.18976 U.11464 C.06808 O.03941 O.02215 O.01646 O.01220 O.00674 O.00010 O.00010 O.00010 O.00011	0.76760 0.57251 0.30248 0.19934 0.20914 0.19861 0.09548 0.03756 0.00523 - C.01011 -0.01533 -0.01526 -0.01298 -0.00375 -0.00102 -0.00173 -0.00102 -0.00007	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135 0.08581 0.04264 0.03145 0.02703 0.02317 0.01684 0.01203 0.00475 0.00042 0.00000	0.57396 0.38767 0.26014 0.21669 0.18150 0.09470 0.06970 0.04853 0.02660 0.01287 0.00598 0.00281 0.00007 -0.00008 -0.00008	0.59596 0.48550 0.46368 0.43307 0.39737 0.10133 0.05753 0.03780 0.03128 0.02581 0.01735 0.01148 0.00381 0.00107 0.00015 -0.00015
1.8 2.0 2.2 2.3 2.6 2.8 3.0 3.2 3.4 3.5 3.6 3.8 4.0 5.0 5.5 6.0	0.59C36 0.483d7 0.45371 0.38026 0.30725 0.11579 0.06423 0.03845 0.02129 0.01425 0.00971 0.00104 -0.00089 -0.00084 -0.00064 -0.00046	0.72444 0.65267 C.49053 0.45984 C.46294 0.29095 0.20045 0.09742 0.09742 0.0852 0.04854 0.04834 0.03414 0.00607 0.00607 0.00607 0.00125	0.50684 0.32532 C.20859 0.17509 C.15253 0.12935 0.11408 C.07824 0.05342 0.05342 0.05490 0.00495 0.00495 0.00495 0.00495 0.00495 0.00495	0.38172 0.24879 0.23629 0.24471 0.08402 0.00285 -0.03285 -0.02529 -0.02194 -0.01865 -0.00378 -0.00378 -0.000378 -0.00052 -0.00065 -0.00086	0.39743 C.29786 0.24489 C.29205 0.25949 0.18976 0.03941 0.02215 0.01646 0.01220 0.00674 0.00380 0.00091 0.00010	0.76760 0.57251 0.30248 0.19934 0.20914 0.03556 0.00523 -C.01011 -0.01533 -0.01533 -0.01526 -0.00225 -0.00173 -0.00102 -0.00102 -0.00102 -0.00030	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135 0.08581 0.02703 0.02703 0.02317 0.01684 0.01203 0.00475 0.00040 0.00000 0.000000	0.57396 0.38767 0.26014 0.21669 0.18150 0.12955 0.09470 0.04853 0.02660 0.01287 0.00598 0.00281 0.00008 -0.00008 -0.00008 -0.00008	0.59596 0.48550 0.46368 0.43307 0.39737 0.17539 0.10133 0.05753 0.03780 0.03780 0.02581 0.01735 0.01188 0.00107 0.00015 -0.00013
1.8 2.0 2.2 2.3 2.6 2.8 3.0 3.2 3.4 3.5 6.5 7.0 7.0	0.59C16 0.485d7 0.453d7 0.38026 0.30725 0.19072 0.0125 0.03845 0.02J29 0.01425 0.0071 0.0039 -0.00084 -0.00064 -0.00046 -0.00046	0.72444 0.65267 C.49053 0.45984 C.46294 0.29095 0.20045 0.13924 0.09742 0.08166 0.06852 0.04834 0.01431 0.00607 0.00267 0.00125 0.00021 0.00021	0.50684 0.32532 C.20859 0.17509 C.15253 0.11408 C.2935 C.12353 0.11408 C.27824 0.05342 0.03616 C.2241b 0.01590 0.00195 0.00195 0.00105 0.00052 -C.00052	0.38172 0.24879 0.24879 0.24471 0.20847 0.03843 -0.03235 -0.02529 -0.01885 -0.01355 -0.00378 -0.00165 -0.00032	0.39743 C.25746 O.24489 C.25949 O.18976 U.11464 C.06808 O.03941 O.02215 O.01646 O.01220 O.00674 O.00010 O.00010 O.00010 O.00011	0. 76760 0. 57251 0. 30248 0. 19934 0. 20914 0. 03756 0. 00523 -0. 01523 -0. 01533 -0. 01526 -0. 01298 -0. 00102 -0. 00102 -0. 00103 -0. 00103 -0. 00103 -0. 00103 -0. 00030	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135 0.08581 0.0959 0.04264 0.03145 0.02317 0.01684 0.01203 0.00475 0.00042 0.000000	0.57396 0.38767 0.26014 0.21669 0.18150 0.12955 0.09470 0.06970 0.04853 0.02660 0.01287 0.00598 0.00281 0.00008 -0.00007 -0.00008 -0.00007 -0.00008	0.59596 0.48550 0.46368 0.43307 0.39737 0.17539 0.10133 0.05753 0.03780 0.03128 0.02581 0.01735 0.01148 0.00181 0.00107 0.00015 -0.00013 -0.00015 -0.00015
1.8 2.0 2.2 2.3 2.4 2.6 2.8 3.0 3.2 3.5 3.6 3.6 3.6 3.6 5.5 5.0 6.0 6.5 7.5	0.59C16 0.485d7 0.45371 0.38026 0.30725 0.19072 0.06123 0.03845 0.02029 0.01425 0.00104 0.00089 -0.00084 -0.00084 -0.00033 -0.00123	0.72444 0.65267 C.49053 0.45984 C.46294 0.29095 0.20045 0.13924 0.08166 0.06852 0.04834 0.01431 0.01431 0.01267 0.00267 0.00126 0.00036	0.50684 0.32532 C.20859 0.17509 C.15253 0.12935 0.11408 0.07842 0.07842 0.03616 C.0241b 0.01590 0.00495 0.00495 0.00052 -C.00054 -C.00054 -0.00049	0.38172 0.24879 0.23629 0.24471 0.20847 0.0402 0.0285 -0.03843 -0.03235 -0.02529 -0.01885 -0.01355 -0.00949 -0.0165 -0.00052 -0.00052 -0.00052 -0.00032 -0.00032 -0.00032	0.39743 C.29786 0.28489 C.29205 0.25949 0.18976 0.11464 0.06808 0.03941 0.02215 0.01646 0.01220 0.00674 0.00380 0.00010 -0.00011 -0.00014 -0.00014	0.76760 0.57251 0.30248 0.19934 0.20914 0.09548 0.03756 0.00523 -C.01011 -0.01533 -0.01523 -0.01298 -0.00325 -0.00173 -0.00102 -0.00011	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135 0.08581 0.05909 0.04264 0.02703 0.02317 0.01624 0.01203 0.00475 0.00042 0.000047 0.000012 0.00012 0.00012	0.57396 0.38767 0.26169 0.18150 0.12955 0.09470 0.06873 0.02660 0.01287 0.00598 0.00281 0.00008 -0.00007 -0.00008 -0.00002 -0.00002	0.59596 0.48550 0.46368 0.43307 0.39737 0.28989 0.17539 0.05753 0.03780 0.03128 0.02581 0.01735 0.01148 0.00381 0.00107 0.00015 -0.00019 -0.00019 -0.00019
1.8 2.0 2.2 2.3 2.4 2.6 3.0 3.2 3.5 3.6 4.0 4.5 6.5 7.0 7.5 8.0	0.59C36 0.483d7 0.45371 0.38626 0.30725 0.19072 0.06423 0.03845 0.02129 0.01425 0.0071 0.00394 0.00104 -0.00089 -0.00084 -0.00033 -0.00023 -0.00016	0.72444 0.65267 C.49053 0.45984 C.46294 0.29095 0.20045 0.13924 0.09742 0.08166 0.06852 0.04834 0.01431 0.00607 0.00267 0.00125 0.00021 0.00021	0.50684 0.32532 C.20859 0.17509 C.15253 0.12935 C.12353 0.11408 C.07824 0.05342 0.05342 0.05490 0.00495 0.00495 0.00495 0.00000000000000000000000000000000000	0.38172 0.24879 0.23629 0.24471 0.08402 0.00285 -0.03285 -0.02529 -0.02194 -0.01865 -0.00949 -0.00052 -0.00052 -0.00052 -0.00052 -0.000052 -0.00002	0.39743 C.29786 0.24489 C.29205 0.25949 0.18976 0.11464 C.06808 0.03941 0.02215 0.01646 0.1220 0.00674 0.00380 0.00091 0.00010 -0.00011 -0.00014 -0.00013 -0.00014	0. 76760 0. 57251 0. 30248 0. 19934 0. 20914 0. 03756 0. 00523 -0. 01523 -0. 01533 -0. 01526 -0. 01298 -0. 00102 -0. 00102 -0. 00103 -0. 00103 -0. 00103 -0. 00103 -0. 00030	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135 0.08581 0.0959 0.04264 0.03145 0.02317 0.01684 0.01203 0.00475 0.00042 0.000000	0.57396 0.38767 0.26014 0.21669 0.18150 0.12955 0.09470 0.06970 0.04853 0.02660 0.01287 0.00598 0.00281 0.00008 -0.00007 -0.00008 -0.00007 -0.00008	0.59596 0.48550 0.46368 0.43307 0.39737 0.17539 0.10133 0.05753 0.03780 0.03128 0.02581 0.01735 0.01148 0.00181 0.00107 0.00015 -0.00013 -0.00015 -0.00015
1.8 2.0 2.2 2.3 2.6 2.8 3.5 3.6 3.5 3.6 4.5 5.5 6.0 7.5 8.0	0.59C16 0.485d7 0.453d7 0.38e26 0.30725 0.19072 0.06423 0.03845 0.02)29 0.01425 0.00471 0.00394 0.00104 0.00089 -0.00084 -0.00346 -0.00346 -0.00346 -0.00016	0.72444 0.65267 C.49053 0.45984 C.46294 0.29095 0.20045 0.13924 0.09742 0.08166 0.06852 0.04834 0.03414 0.01431 0.00607 0.00267 0.00025 0.00021 0.00012	0.50684 0.32532 C.20859 0.17509 C.15253 0.11408 C.67824 0.05342 0.03616 C.02418 0.0159 0.00109 0.000022 -C.00049 -C.00049 -C.00049 -C.00049 -C.00049 -C.00049 -C.00049	0.38172 0.24879 0.23629 0.24471 0.20847 0.03843 -0.03235 -0.02529 -0.02194 -0.01885 -0.03949 -0.00376 -0.00096 -0.00092 -0.00092 -0.00007 -0.00007	0.39743 C.25746 0.24489 C.25949 0.18976 0.11464 0.06808 0.03941 0.02215 0.01646 0.01220 0.00674 0.00010 0.00010 -0.00011 -0.00013 -0.00013 -0.00013 -0.00019 -0.000019 -0.000019 -0.000019 -0.000019	0.76760 0.57251 0.30248 0.19934 0.20914 0.09548 0.03756 0.00523 -C.01011 -0.01533 -0.01523 -0.01298 -0.00325 -0.00173 -0.00102 -0.00011	0.70054 0.50662 0.33331 0.26410 0.20858 0.13135 0.08581 0.05909 0.04264 0.02703 0.02317 0.01624 0.01203 0.00475 0.00042 0.000047 0.000012 0.00012 0.00012	0.57396 0.38767 0.26169 0.18150 0.12955 0.09470 0.06873 0.02660 0.01287 0.00598 0.00281 0.00008 -0.00007 -0.00008 -0.00002 -0.00002	0.59596 0.48550 0.46368 0.43307 0.39737 0.28989 0.17539 0.05753 0.03780 0.03128 0.02581 0.01735 0.01148 0.00381 0.00107 0.00015 -0.00019 -0.00019 -0.00019

Tabular Data. A-14.4 Calculated potential curves for 62 valence states of 0_2 given in hartrees relative to the asymptotic energy of each state. (Continued).

R(a ₀)	4¹ Π _u	$a^1 \Delta_g$	$2^1\Delta_g$	31 Ag	$4^1\Delta_g$	1 1 A	$2^1\Delta_u$	¹ Ф _g	100
1.8	0.54772	0. 27303	0.44183	0.81141	0.78295	0.52510	0.53453	0.39220	0.64196
2.0	0.44275	-0.07635	C.33837	0.59776	0.53975	0.26985	0.42168	0.29999	0.53868
2.2	0:38046	-0.13196	0.31716	0.36249	0.46403	0.12428	0.38110	0.28713	0.51136
2.3	0.35327	-C. 14051	C.27576	0.32183	0.44640	0.07721	0.35421	0.29497	0.49255
2.4	0.33574	-0.14133	0.21382	0. 33185	0.38321	C. C4198	0.31217	0.26490	0.47536
2.6	0.23706	-0.12912	0.11913	0.31593	0.26336	-0.00292	0.23946	0.14653	0.34171
2.8	0.15418	-0.10807	0.05918	0.20517	C. 29479	- C. 02485	0.19071	0.07417	0.22628
3.0	0.09571	-0.08492	0.02210	0.13171	0.22231	-0.03269	0.14287	C. C3210	0.14980
3.2	0.05738	-0.06333	0.00030	0.08396	0.14570	-0.03239	0.09062	0.00923	0.09934
3.4	0.03406	-0.04520	-0.01113	0.05345	0.09402	-0.02799	0.05623	-0.00193	0.06610
3.5	0.02641	-0.03767	-0.01406	0.04271	0.07511	0.02512	0.04402	-0.00474	0.05401
3. 5	0.02361	-0.03118	-C.01560	0.03418	0.05978	-0.02214	0.03432	-0.00633	0.04419
3.8	0.01286	-0.02106	-0.01576	0.02202	0.03750	-0.01647	0.02062	-0.00719	0.02967
4.0	0.00835	-0.01412	-C.01371	0.01428	0.02328	-0.01182	0.01223	-0.0C651	0.02000
4.5	0.00337	-0.00538	-0.00730	0.00488	0.00707	-0.00516	0.00326	-0.00387	0.00750
5.0	0.00161	-0.00222	-0.00354	0.00163	0.00232	-0.00263	0.00085	-0.00230	0.00280
5.5	0.00083	-0.00099	-0.00184	0.00051	0.00082	-0.00153	0.00013	-0.00147	0.00103
6.0	0.00046	-0.00048	-0.00105	0.00014	0.00030	-0.00097	-0.00008	-0.00099	0.00038
6.5	0.00029	-0.00026	-0.00066	0.30002	0.00011	- 0. CC065	-0.00013	-0.00068	0.00014
7.0	0.00018	-0.00014	-0.00043	-0.00001	0.00004	-0.00044	-0.00012	-0.00048	0.00005
7.5	0.00713	-0.00008	-0.00029	-0.00002	C. 0CC01	-0.00031	-0.00010	-0.00034	0.00002
8.0	0.00009	-0.00005	-C.0002C	-0.00001	0.00000	-0.00022	-0.00007	-0.00024	0.00001
9.0	0.00105	-0.00002	-0.00010	-0.00001	0.00000	-C.00011	-0.00004	-0.00013	0.00001
10.0	0.00003	-0.0000C	-C.00C05	-0.00000	0.00000	-0.00006	-0.00002	-0.00007	0.00001
20.0	0.26233	0.00000	0.16597	0.16600	0.26239	0.16597	0.26239	0. 16612	0.16612

R(a ₀)	11°g	3 ½ ⁺ ₉	×3Σ-g	$2^3\Sigma_{g}$	3 ³ Σ-	4 ³ \(\Sigma_g^-\)	A35,	5 ₃ Σ ⁿ +	3 ³ Σ ₊ ,
1.8	0.85720	0.48328	C.C2825	0.50430	0.81931	0.80922	0.50973	0.77601	0.83606
2.0	0.68188	0. 38790	-0.12072	0.40243	0.61562	0.55214	0.24316	0.67036	0.69923
2.2	0.60357	0.37171	-C.17448	0.38002	0.38406	0.48151	0.09950	0.59077	0.56181
2.3	0.59368	0.37819	-0. 18 168	0.30006	0.38657	C. 45847	0.05574	0.49613	0.56036
2.4	0.58057	0.38975	-0.18093	0.23430	0.39556	0.35303	0.02465	0.41659	0.54220
2.6	0.54370	0.35125	-0.16494	0.13940	0.28995	C. 32792	-0.01125	0.29756	0.38770
2.8	0.37589	0.23825	-0.13934	0.07840	0.18311	0. 27285	-0.02517	0.21796	0.24472
3.0	0.25/42	0.16139	-0.11081	0. C3906	0.11287	0.20421	-0.02711	0.16473	0.14581
3.2	0.17646	C. 10925	-0.08304	0.01339	0.06801	0.13845	-0.02319	0.12943	0.07716
3.4	0.12114	0.07392	-0.05925	-0.00343	C. C4048	C.08888	-0.01724	0.10663	0.02935
3.5	0.10043	0.06080	-0.04743	-0.00930	0.03122	0.07045	-0.01425	0.09283	0.01709
3.6	0.08330	0.05000	-0.03787	-0.01366	C-C2413	0.05548	-0.01151	0.07763	0.01107
3.8	0.05738	0.03378	-C-C2278	-0.01829	0.01447	0.03371	-0.00709	0.05427	0.00339
4.0	0.03357	0.02278	-0.C1300	-0.01348	0.00866	0.01994	-0.00417	0.03794	-0.00029
4.5	0.01571	0.00841	-0.C0354	-0.01110	0.00210	0.00493	-0.00123	0.01554	-0.00189
5.0	0.00233	0.00304	-0.00145	-0.00515	0.00010	C. CC118	-0.00056	0.00642	-0.00110
5.5	0.00262	0.00106	-C.0CC78	-0-00235	-0.00043	0.00024	-0.00033	0.00272	-0.00052
6.0	0.00114	0. 30035	-0.00047	-0.00111	-0.00051	-0.00002	-0.00021	0.00119	-0.00024
6.5	0.00053	0.00010	-0.00030	-0.00055	-0.00047	-0.00009	-0.00013	0.00055	-0.00012
7.0	0.00128	0.00002	-0.00019	-0.00028	-0.00039	- C. CCC09	-0.00007	0.00027	-0.00006
7.5	0.00016	-0.00000	-C.00C13	-0.00015	-0.00030	-0.00008	-0.00004	0.00015	-0.00003
8.0	0.00010	-0.00000	-0.00008	-0.00009	-0.00022	- 0. CCC06	-0.00002	0.00009	-0.00001
9.0	0.00005	0.00000	-C.00C03	-0.00004	-0.00011	-0.00003	0.00000	0.00004	-0.00000
10.0	0.00003	0.00000	-0.00001	-0.00002	-0.CC006	-0.00001	0.00001	0.00003	0.00000
20.0	0.16025	0.08300	-c.cocco	0.04300	0.08345	C. 17974	0.00000	0.00125	0.08300

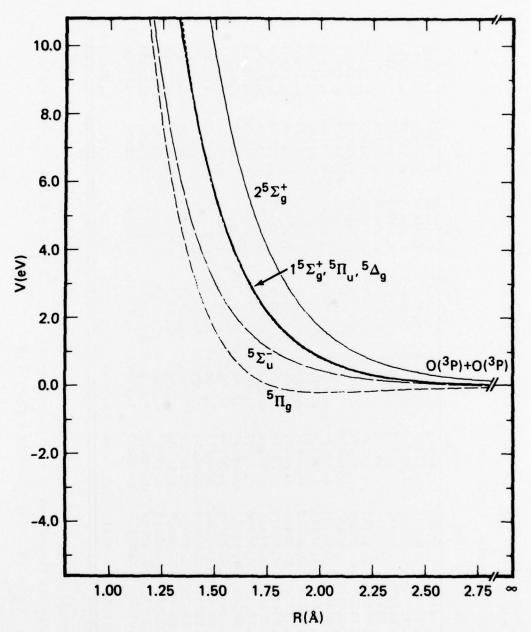
Tabular Data. A-14.4 Calculated potential curves for 62 valence states of θ_2 given in hartrees relative to the asymptotic energy of each state. (Continued).

R(a ₀)	$8^3\Sigma_u^-$	23 5 u	$3^3\Sigma^{\alpha}$	1 ³ 11 ₉	2 ³ 11 _g	3 ³ 11 _g	4 ³ 11 _g	5 ³ 11 _g	13II _u
1.8	0.51595	0.69461	0.74252	0.43650	0.42217	C.46823	0.89067	0.85222	0.63719
2.0	0.25852	0.58419	C.59300	0.26433	0.32404	0. 37538	0.69775	0.61916	0.44513
2.2	0.11369	0.50650	0.44503	0.15112	0.31672	C. 36241	0.42547	0.38047	0.27091
2. 1	0. 06710	0.41117	C.4C759	0.11872	0.32361	0. 12540	0. 366 10	0.28031	0.20252
2.4	0.03210	0.13260	0.36182	0.01685	0.24153	C.28681	0.33320	0.24330	0.14870
2.6	-0.01199	0.21813	C.29C80	0.97389	0.12419	0. 16 38 7	0.21717	0. 22581	0.07620
2.8	-0.03361	0.14454	0.24239	0.05692	0.05160	0.08651	0.14436	0.12997	0.03660
3.0	-0.04126	0.09709	0.16851	0.06717	0.00710	0.03962	0.09844	0.06733	0.01705
3.2	-0.04365	0.06605	0.10917	0.06038	-C.01129	0.01297	0.06790	0.03005	0.00887
3.4	-0.03566	0.04532	0.06914	0.04210	-0.00850	-0.00054	0.04633	0.01074	0.00631
3.5	-0.03237	0. 0 3761	0.05445	0.03513	-0.CC726	-0.00397	0.03804	0.00549	0.00592
3.6	-0.02888	0.03122	0.04254	0.02930	-0.C0680	-0.00513	0.03113	0.00213	0.00571
3.8	-0.02202	0.02147	0.02529	0.02026	-0.00758	-0.00401	0.02074	-0.00108	0.00516
4.0	-0.01608	0.01465	0.01452	0.01391	-0.00692	-0.00276	0.01375	-0.00190	0.00412
4.5	-0.00687	0.00525	0.00330	0.00510	-0.00384	-0.00121	0.00474	-0.00137	0.00114
5.0	-0.00311	0.00152	0.00075	0.00164	-0.00194	-0.00070	0.00144	-0.00077	-0.00036
5.5	-0.00153	0.00014	0.00012	0.00038	-0.00101	-0.00C52	0.00028	-0.00047	-0.00075
6.0	-0.00078	-0.00032	-C.COC05	-0.00002	-0.00051	-0.00044	-0.00009	-0.00031	-0.00071
6.5	-0.00039	-0.00043	-0.00010	-0.00013	-0.00023	-0.00039	-0.00019	-0.00021	-0.00057
7.0	-0.00020	-0.00039	-0.00009	-0.00013	-0.00009	-0.00031	-0.00018	-0.00014	-0.00042
7.5	-0.00)12	-0.00030	-0.00008	-0.00010	-0.00005	-0.00021	-0.00015	-0.00010	-0.00031
8.0	-0.00008	-0.00022	-0.00006	-0.10008	-0.C0003	-0.C0014	-0.00012	-0.00006	-0.00022
9.0	-0.00004	-C.00011	-0.00003	-0.00004	-0.00000	-0.00007	-0.00007	-0.00003	-0.00012
10.0	-0.00002	-0.00006	-0.00001	-0.00002	0.00001	-0.00003	-0.00004	-0.00001	-0.00006
20.0	0.68300	0.08345	0. 17974	0.30062	0.08235	0.08312	0.08360	0.17924	0.00061
R(a ₀)	2 ³ 11 ₀	3 ³ II _u	4 ³ П _U	5 ³ П _и	$1^3\Delta_{q}$	$2^3\Delta_{ m g}$	$C^3\Delta_{_U}$	2 ³ Δ ₀	$3^3\Delta_{_{\scriptscriptstyle U}}$
1.8	0.53440	0.65994	0.71111	0.75055	0.47807	C.87063	0.50075	0.68513	0.8.344
2.0	0.40706	0.55385	C.60C59	0.51157	0.38295	0.70058	0.23574	0.58003	0.69787
2.2	0.31432	0.41100	0.52034	0.43980	0.36679	0.62815	0.09337	0.48618	0.55229
2.3	0.28349	0.35716	C.49528	0.42641	0.37333	0.60569	0.05019	0.38976	0.55091
2.4	0.24738								
2.6		0.33122	0.47765	0.39673	0.38494	C.50823	0.01962	0.31071	
	0.17747	0.33122	0.47765	0.25337	0.34655	0.41475	0.01962		0.54000
2.8	0.17747							0.31071	
3.0		0.30900	C.32361	0.25337	0.34655	0.41475	-0.01537	0.31071	0.54000
3.0	0.12552	0.30900	0.32361	0.25337	0.34655	0.41475 C.37807	-0.01537 -0.02855	0.31071 0.19487 0.11941	0.54008 0.44992 0.31130
3. 0	0.12552 0.08777	0.30900 0.19872 0.12014	0.32361 0.23133 0.15366	0.25337 0.17971 0.11638	0.34655 0.23456 0.15840	0.41475 0.37807 0.25955	-0.01537 -0.02855 -0.02989	0.31071 0.19487 0.11941 0.07025	0.54008 0.44992 0.31130 0.21627
3. 0 3. 2 3. 4 3. 5	0.12552 0.08777 0.05378	0.30900 0.19872 0.12014 0.06959	0.32361 0.23133 0.15366 0.10220	0.25337 0.17971 0.11638 0.07269 0.04503 0.03539	0.34655 0.23456 0.15840 0.10681	0.41475 0.37807 0.25955 0.17837	-0.01537 -0.02855 -0.02989 -0.02550	0.31071 0.19487 0.11941 0.07025 0.03843	0.5400d 0.44992 0.31130 0.21627 0.15088
3.0 3.2 3.4	0.12552 0.08777 0.05578 0.03208	0.30900 0.19872 0.12014 0.06959 0.04325	0.32361 0.23133 0.15366 0.10220 0.06804	0.25337 0.17971 0.11638 0.07269 0.04503	0.34655 0.23456 0.15840 0.10681 0.07191	0.41475 0.37807 0.25955 0.17837 3.12276	-0.01537 -0.02855 -0.02989 -0.02550 -0.01916	0.31071 0.19487 0.11941 0.07025 0.03843 0.01839	0.54008 0.44992 0.31130 0.21627 6.15088 0.10555
3. 0 3. 2 3. 4 3. 5	0.12552 0.08777 0.05378 0.03208 0.02136	0.30900 0.19872 0.12014 0.06959 0.04325 0.03505 0.02844 0.01859	0.32361 0.23133 0.15366 0.10220 0.06804 0.05553	0.25337 0.17971 0.11638 0.07269 0.04503 0.03539	0.34655 0.23456 0.15840 0.10681 0.07191 0.05896	0.41475 0.37807 0.25955 0.17837 3.12276 0.10190	-0.01537 -0.02855 -0.02989 -0.02550 -0.01916 -0.01601	0.31071 0.19487 0.11941 0.07025 0.03843 0.01839	0.54008 0.44992 0.31130 0.21627 0.15088 0.10555 0.08835
3. 0 3. 2 3. 4 3. 5 3. 6	0.12552 0.08777 0.05878 0.03208 0.02136 0.01314	0.30900 0.19872 0.12014 0.06959 0.04325 0.03505 0.02844	0.32361 0.23133 0.15366 0.10220 0.06804 0.05553 0.04532	0.25337 0.17971 0.11638 0.07269 0.04503 0.03539 0.02779	0.34655 0.23456 0.15840 0.10681 0.07191 0.05896 0.04832	0.41475 0.37807 0.25955 0.17837 3.12276 0.10190 0.08462	-0.01537 -0.02855 -0.02989 -0.02550 -0.01916 -0.01601 -0.01311	0.31071 0.19487 0.11941 0.07025 0.03843 0.01839 0.01161 0.00652	0.54008 0.44992 0.31130 0.21627 0.15088 0.10555 0.08835 0.07397
3.0 3.2 3.4 3.5 3.6 3.8 4.0 4.5	0.12552 0.08777 0.05478 0.03208 0.02136 0.01314 0.00293 -0.00155 -0.00288	0.30900 0.19872 0.12014 0.06959 0.04325 0.03505 0.02844 0.01859 0.01200 0.00372	C.32361 O.23133 C.15366 O.10220 C.06804 O.05553 O.04532 Q.03016 C.02C03 O.00703	0.25337 0.17971 0.11638 0.07269 0.04503 0.03539 0.02779 0.01707 0.01042 0.00290	0.34655 0.23456 0.15840 0.1681 0.07191 0.05896 0.04832 0.03239 0.02162 0.00764	0.41475 C.37807 0.25955 0.17837 J.12276 0.10190 0.08462 0.05842 0.04040 0.01619	-0.01537 -0.02855 -0.02989 -0.02550 -0.01916 -0.01601 -0.01311 -0.00841	0.31071 0.19487 0.11941 0.07025 0.03843 0.01161 0.00652 0.00025	0.54008 0.44992 0.31130 0.21627 0.15088 0.10555 0.08835 0.07397 0.05187
3.0 3.2 3.4 3.5 3.6 3.8 4.0 4.5 5.0	0.12552 0.08777 0.05978 0.03208 0.02136 0.01314 0.00293 -0.00155 -0.00288 -0.00174	0.30900 0.19872 0.12014 0.06959 0.04325 0.03505 0.02844 0.01859 0.01200 0.00372 0.00091	0.32381 0.23133 0.15366 0.10220 0.06804 0.05553 0.04532 0.03016 0.02003	0.25337 0.17971 0.11638 0.07269 0.04503 0.03539 0.02779 0.01707 0.01042 0.00290 0.0067	0.34655 0.23456 0.15840 0.10681 0.07191 0.05896 0.04832 0.03239 0.02162 0.00764 0.00252	0.41475 0.37807 0.25955 0.17837 3.12276 0.10190 0.08462 0.05842 0.04040 0.01619 0.00662	-0.01537 -0.02855 -0.02989 -0.02550 -0.01916 -0.01601 -0.01311 -0.00841 -0.00525	0.31071 0.19487 0.11941 0.07025 0.03843 0.01161 0.00652 0.00025	0.54008 0.44992 0.31130 0.21627 0.15088 0.10555 0.08835 0.07397 0.05187 0.03639
3.0 3.2 3.4 3.5 3.6 3.8 4.0 4.5 5.0	0.12552 0.08777 0.05378 0.03208 0.02136 0.01314 0.00293 -0.00155 -0.0028 -0.00174 -0.00396	0.30900 0.19872 0.12014 0.06959 0.04325 0.03505 0.02844 0.01859 0.01200 0.00372 0.00091	C.32361 O.23133 C.15366 O.10220 C.06804 O.05553 O.04532 Q.03016 C.02C03 O.00703	0.25337 0.17971 0.11638 0.07269 0.04503 0.03539 0.02779 0.01707 0.01042 0.00290	0.34655 0.23456 0.15840 0.10681 0.07191 0.05896 0.04832 0.023239 0.02162 0.00764 0.00252 0.00071	0.41475 C.37807 0.25955 0.17837 J.12276 0.10190 0.08462 0.05842 0.04040 0.01619 0.00662 0.00279	-0.01537 -0.02855 -0.02955 -0.02550 -0.01916 -0.01601 -0.01311 -0.00841 -0.00525 -0.00180	0.31071 0.19487 0.11941 0.07025 0.03843 0.01839 0.01161 0.00652 -0.0025 -0.00250	0.54008 0.44994 0.31130 0.21627 6.15088 0.10555 0.08835 0.07397 0.05187 6.03639
3.0 3.2 3.4 3.5 3.6 3.8 4.0 4.5 5.0 5.5 6.0	0.12552 0.08777 0.05478 0.03208 0.02136 0.01314 0.00293 -0.00155 -0.00288 -0.00174 -0.00096	0.30900 0.19872 0.12014 0.06959 0.04325 0.03505 0.02844 0.01859 0.01200 0.00372 0.00091 1.00000	C.32381 O.23133 C.15366 O.10220 C.06804 O.05553 O.04532 O.03016 C.02C03 O.00703 O.00229	0.25337 0.17971 0.11638 0.07269 0.04503 0.03539 0.02779 0.01707 0.01042 0.00290 0.0067	0.34655 0.23456 0.15840 0.10681 0.07191 0.05896 0.04832 0.03239 0.02162 0.00764 0.00252	0.41475 0.37807 0.25955 0.17837 3.12276 0.10190 0.08462 0.05842 0.04040 0.01619 0.00662	-0.01537 -0.02855 -0.02950 -0.02550 -0.01916 -0.01601 -0.01311 -0.00841 -0.00525 -0.00180 -0.0084	0.31071 0.19487 0.11941 0.07025 0.03843 0.01181 0.00652 0.00025 -0.00250 -0.00292	0.5400d 0.44992 0.31130 0.21627 6.15088 0.10555 0.08835 0.07397 0.03637 0.03637 0.03637
3. 0 3. 2 3. 4 3. 5 3. 6 3. 8 4. 0 4. 5 5. 0 5. 5 6. 0 6. 5	0.12552 0.08770 0.05478 0.03208 0.02136 0.01314 0.00293 -0.0015 -0.00288 -0.00174 -0.00096 -0.00051	0.30900 0.19872 0.12014 0.06959 0.04325 0.02844 0.01859 0.01200 0.00372 0.00091 0.000027 -0.00027	C.32381 0.23133 0.15366 0.10220 0.06804 0.05553 0.04532 0.03016 0.00203 0.00703 0.00229 0.00003 -C.00C14	0.25337 0.17971 0.11638 0.07269 0.04503 0.03539 0.02779 0.01042 0.00290 0.30067 0.000015 -0.00015	0.34655 0.23456 0.15840 0.10681 0.07191 0.05896 0.04432 0.03239 0.02162 0.00764 0.00252 0.00071	0.41475 0.37807 0.25955 0.17837 3.12276 0.10190 0.08462 0.05842 0.04040 0.01619 0.0062 0.00279 0.00123 0.00123	-0.01537 -0.02855 -0.02989 -0.02550 -0.01916 -0.01601 -0.01311 -0.00525 -0.00180 -0.00084 -0.00089 -0.00099	0.31071 0.19487 0.11941 0.07025 0.03839 0.01161 0.00652 0.00025 -0.00250 -0.00250	0.5400d 0.4499d 0.31130 0.21627 0.1508d 0.10555 0.08835 0.07397 0.05187 0.03639 0.01499 0.00623 0.00266
3. 0 3. 2 3. 4 3. 5 3. 6 3. 8 4. 0 4. 5 5. 5 6. 0 6. 5 7. 0	0.12552 0.08777 0.05378 0.03208 0.02136 0.01314 0.00293 -0.00155 -0.00288 -0.00174 -0.00051 -0.00053	0.3090C 0.19872 0.12014 0.06959 0.04325 0.03505 0.01200 0.01200 0.00372 0.00091 0.00000 -0.00027 -0.00030	C.32361 2.23133 C.15366 2.10220 C.06804 0.05553 0.04532 0.03016 C.02203 0.00703 0.00229 0.00060 0.00003 -C.00C14 -0.00017	0.25337 0.17971 0.11638 0.07269 0.04503 0.03539 0.02779 0.01707 0.01042 0.00290 0.00001 -0.00015 -0.00015	0.34655 0.23456 0.15840 0.10681 0.07191 0.05896 0.04432 0.02162 0.00764 0.00252 0.00071 0.00012 -0.00008	0.41475 0.37807 0.25955 0.17837 0.10190 0.08462 0.05842 0.04040 0.01619 0.00662 0.00279 0.00123 0.00028	-0.01537 -0.02855 -0.02989 -0.02550 -0.01916 -0.01601 -0.00341 -0.00525 -0.00180 -0.00084 -0.00048 -0.00029 -0.00012	0.31071 0.19487 0.11941 0.07025 0.03843 0.01161 0.00652 0.00025 -0.00250 -0.00250 -0.00167 -0.00087	0.5400a 0.44992 0.31130 0.21627 0.15080 0.10555 0.08835 0.07397 0.05187 0.03639 0.01499 0.00623 0.0026
3.0 3.4 3.5 3.6 3.8 4.0 4.5 5.5 6.0 6.5 7.0	0.12552 0.08777 0.05378 0.03208 0.02136 0.01314 0.00293 -0.00155 -0.00288 -0.00174 -0.00096 -0.00051 -0.00023	0.3090C 0.19914 0.12014 0.06959 0.04325 0.03505 0.01200 0.0037 0.00091 0.00091 0.00027 -0.00032 -0.00031	C.32361 2.23133 C.15366 2.10220 C.06804 0.05553 0.04532 0.03703 0.00703 0.00229 0.00600 -C.00C014 -0.00017 -0.00015	0.25337 0.17971 0.11638 0.04503 0.04503 0.03539 0.02779 0.01042 0.00297 0.00001 -0.00015 -0.00015	0.34655 0.23456 0.15840 0.10681 0.07191 0.05896 0.04432 0.03239 0.02162 0.00764 0.00252 0.00071 -0.00005 -0.00005	0.41475 0.37807 0.25955 0.17837 0.10190 0.08462 0.05842 0.04040 0.01619 0.00662 0.00279 0.00123 0.00058 0.00029	-0.01537 -0.02855 -0.02989 -0.02550 -0.01916 -0.01601 -0.03841 -0.00525 -0.00180 -0.00084 -0.00084 -0.00089 -0.00089 -0.00019 -0.00019	0.31071 0.19487 0.11941 0.07025 0.03843 0.01839 0.01161 0.00652 0.00025 -0.0025 -0.00292 -0.00167 -0.00087 -0.00027 -0.000167	0.54004 0.44992 0.31130 0.21627 0.15080 0.10555 0.0835 0.07397 0.05187 0.03639 0.01099 0.00623 0.00119 0.00059 0.00029
3.0 3.2 3.4 3.5 3.6 4.0 4.5 5.0 5.5 6.0 7.5	0.12552 0.08777 0.05478 0.02136 0.02136 0.01314 0.00293 -0.00155 -0.00288 -0.00174 -0.00091 -0.00093 -0.00008	0.3090C 0.19214 0.12014 0.06959 0.04325 0.03505 0.01200 0.0037 0.00091 0.00027 -0.00023 -0.00023 -0.00021 -0.00023	C.32361 2.23133 C.15366 2.10220 C.06804 0.05553 0.04532 0.03703 0.00703 0.00229 C.00C60 0.00003 -C.00C14 -O.00C17 -O.00015	0.25337 0.17971 0.11638 0.07269 0.04503 0.03539 0.02779 0.01042 0.00290 0.00001 -0.00015 -0.00015 -0.00012	0.34655 0.23456 0.15840 0.10681 0.07191 0.05896 0.04432 0.03239 0.02162 0.00764 0.00252 0.00071 0.00005 -0.00008 -0.00008	0.41475 0.25955 0.17837 3.12276 0.10190 0.08462 0.05842 0.04040 0.01619 0.00662 0.00279 0.00123 0.00058 0.00029 0.00016	-0.01537 -0.02855 -0.02989 -0.02550 -0.01916 -0.01601 -0.03111 -0.00841 -0.00525 -0.00180 -0.00084 -0.00048 -0.00019 -0.00019 -0.00019 -0.00005	0.31071 0.19487 0.11941 0.07025 0.03843 0.01839 0.01161 0.00652 -0.0025 -0.0025 -0.0025 -0.00087 -0.00087 -0.00087 -0.00027	0.54004 0.44992 0.31130 0.21627 0.15084 0.10555 0.05835 0.07397 0.05187 0.03639 0.00623 0.00056 0.0019
3.0 3.2 3.4 3.5 3.6 4.0 4.5 5.0 5.5 6.0 6.5 7.0 7.5 8.0 9.0	0.12552 0.08777 0.05478 0.02136 0.01314 0.00293 -0.00155 -0.00174 -0.00196 -0.00096 -0.00005 -0.00003 -0.00005	0.30900 0.19872 0.12014 0.06959 0.04325 0.03505 0.01200 0.01200 0.00372 0.00091 -0.00030 -0.00030 -0.00031 -0.00001 -0.00001	C.32361 2.23133 C.15366 2.10220 C.06804 0.05553 0.04532 0.03016 C.02203 0.00703 0.00229 0.00060 0.00003	0.25337 0.17971 0.11638 0.07269 0.04503 0.03539 0.02779 0.01707 0.01042 0.00290 0.00015 -0.00015 -0.00015 -0.00016 -0.00004	0.34655 0.23456 0.15840 0.10681 0.07191 0.0252 0.0252 0.00764 0.00252 0.00071 0.00005 -0.00008 -0.00007 -0.00005	0.41475 0.37807 0.25955 0.17837 0.10190 0.08462 0.05842 0.04040 0.01619 0.0062 0.00279 0.0012 0.00029 0.00016 0.00016 0.00005	-0.01537 -0.02855 -0.02989 -0.02550 -0.01960 -0.01601 -0.00341 -0.00525 -0.00180 -0.00048 -0.00048 -0.00029 -0.00012 -0.00007 -0.00007 -0.00007	0.31071 0.19487 0.11941 0.07025 0.03843 0.01839 0.01161 0.00652 0.00025 -0.0025 -0.00292 -0.00167 -0.00087 -0.00087 -0.00007	0.54004 0.44992 0.31130 0.21627 0.15080 0.10555 0.0835 0.07397 0.05187 0.03639 0.01099 0.00623 0.00119 0.00059 0.00029
3.0 3.2 3.4 3.5 3.6 4.0 5.0 5.5 6.0 7.5	0.12552 0.08777 0.05478 0.02136 0.02136 0.01314 0.00293 -0.00155 -0.00288 -0.00174 -0.00091 -0.00093 -0.00008	0.3090C 0.19214 0.12014 0.06959 0.04325 0.03505 0.01200 0.0037 0.00091 0.00027 -0.00023 -0.00023 -0.00021 -0.00023	C.32361 2.23133 C.15366 2.10220 C.06804 0.05553 0.04532 0.03703 0.00703 0.00229 C.00C60 0.00003 -C.00C14 -O.00C17 -O.00015	0.25337 0.17971 0.11638 0.07269 0.04503 0.03539 0.02779 0.01042 0.00290 0.00001 -0.00015 -0.00015 -0.00012	0.34655 0.23456 0.15840 0.10681 0.07191 0.05896 0.04432 0.03239 0.02162 0.00764 0.00252 0.00071 0.00005 -0.00008 -0.00008	0.41475 0.25955 0.17837 3.12276 0.10190 0.08462 0.05842 0.04040 0.01619 0.00662 0.00279 0.00123 0.00058 0.00029 0.00016	-0.01537 -0.02855 -0.02989 -0.02550 -0.01916 -0.01601 -0.03111 -0.00841 -0.00525 -0.00180 -0.00084 -0.00048 -0.00019 -0.00019 -0.00019 -0.00005	0.31071 0.19487 0.11941 0.07025 0.03843 0.01839 0.01161 0.00652 -0.00252 -0.00252 -0.00087 -0.00087 -0.00087 -0.00007 -0.00016	0.5400a 0.44992 0.31130 0.21627 0.15080 0.10555 0.08835 0.07397 0.05187 0.01499 0.00623 0.00119 0.00056 0.00019

Tabular Data. A-14.4 Calculated potential curves for 62 valence states of 0_2 given in hartrees relative to the asymptotic energy of each state. (Continued).

R(a ₀)	$^3\Phi_9$	°Ф.	152°	$2^5\Sigma_9^+$	5 <u>2</u> -	6 U 2	5n _u	$^{5}\Delta_{9}$
1.8	0.46347	0.70406	1.18893	1.32424	0.95557	0.94008	0.91197	0.94106
2.0	3.37205	0.60298	0.95967	1.07451	0.71817	6.71078	0.69442	0.77333
2.2	0.35965	C. 56491	0.73495	0.84102	0.46895	0.43643	0.59166	0-10400
2.3	0.36759	0.53812	0.60427	0.83470	0.37435	C. 33463	0.56513	0.59879
2.4	0.28329	C. 5208C	C. 49597	0.77697	0.29813	0.25320	0.50356	0.49100
2.6	0.17215	0.35281	0.33339	0.55335	0.18901	C. 13835	0.33477	0.32933
2.8	0.10003	0.23510	0.22374	0.38083	0.12005	0.06909	0.22230	C. 22045
3.0	0.05677	0.15615	0.14995	9.26218	C. C7802	C.02909	0.14742	0.14731
3.2	0.03153	0.10333	C. 10C34	0.18071	0.05125	0.00739	0.09759	0.09824
3.4	0.01720	0.06309	0.06705	.0.12472	0.03415	- 0.00325	0.06442	0.06538
3.5	0.01264	0.05518	C.05477	0.10366	0.02799	-0.00546	0.05228	0.05329
3.6	0.00928	0.04465	0.04472	0.03618	0.02238	- 0.00751	0.04238	0.04341
3.8	0.00497	0.02910	0.02576	0.03463	0.01550	-0.00838	0.02774	C. 02874
0.4	0.00260	0.01830	0.01974	0.04131	0.010.0	-0.00772	0.01804	0.01894
4.5	0.00017	0.00591	0.00691	9.01663	0.00354	-0.00486	0.00588	0.00649
5.0	-0.00047	0.00152	0.00231	0.00690	0.00097	- C. 30287	0.00169	0.00209
5.5	-0.00055	9.00014	0.00000	6.00245	0.00010	-0.00174	0.00032	0.00058
0.9	-0.00347	-0.00023	0.00017	0.00124	-0.00014	- 0.00110	-0.00007	6000000
6.5	-0.00035	-C.00027	C.00001	0.30357	-0.00018	-0.00071	-0.00015	-0.00005
7.0	-0.00025	-0.00023	-0.00002	0.33028	-0.00015	- C. COO48	-0.00014	-0.00007
1.5	-0.00018	-0.00017	-0.00002	0.00015	-0.00011	-0.00033	-0.00011	-0.00006
8.0	-0.00013	-0.00012	-0.00001	6000000	-C. CC000	- 0.00023	-0.00008	-0.00004
0.6	96000-0-	-0.00006	0000000	0.00004	-0.00003	-0.00012	10000.0-	-0.00001
10.0	-0.00303	-0.00003	0.00001	0.00003	-0.00001	-0.00000	-0.00002	-0.00000
20.0	0.08312	0.03312	0000000	0.00125	0.00125 -0.00000	0.00061	0.09062	0.0000

energies for R = $20a_0$ are given relative to the calculated 3P + 3P asymptote of -149.695177 hartrees. $1a_0$ = 0.52918 A; 1 hartree = 27.2116 eV. $^{\rm a}$ The asymptotic energy for each state is taken to be the calculated energy at R = $20a_0$. The



Graphical Data. A-14.5. Calculated potential curves for quintet valence states of 0_2 . Energies are given relative to $0\ (^3P)$ + $0\ (^3P)$.

Tabular Data. A-14.6. Molecular constants for 12 electronic states of $\mathbf{0_2}.^{\mathbf{a}}$

State	Ref.	$R_{\sigma}(\text{Å})$	$D_e(eV)$	$D_0(eV)$	$T_e(eV)$	$T_0(eV)$	$\omega_e(\text{cm}^{-1})$	$\omega_e x_e (\text{cm}^{-1})$	$B_e(\text{cm}^{-1})$	$a_e(cm^{-1})$
X3 Σ,	1	1, 236	4.957	4.864		4.	1498.8	9.87	1.38	0.0141
	Exptl, 2	1.208	5.213	5.115			1580.2	11.98	1.45	0.0159
	3	1.30	3.81	3, 72			1582.	14.	1.25	0.0127
	4	1.238	4.876				1692.7			
$a^1\Delta_e$	1	1, 250	3, 857	3,771	1.098	1,091	1403.4	8.74	1,35	0.0158
	Exptl, 2	1,216	4.231	4.138	0.982	0.977	1509.3	12.9	1,43	0.0171
		1.33	2, 81	2.72		1.00	1406.	16,	1, 19	0, 0134
	3	1.249	3.787		1.089		1595.0			0,010.
b 1 Σ;	1	1, 267	3, 168	3.087	1.776	1,764	1310.8	10,44	1, 31	0,0172
28	Exptl. 2	1, 227	3.577	3.489	1.636	1.627	1432.7	13, 93	1, 40	0.0172
	3	1. 34	2.44	2.36	1.050	1.36	1318.	18.	1, 17	
	4	1. 260	3. 185	2.30	1.691	1.30	1505.1	10.	1, 17	0.017
$c^1\Sigma_u^-$	1	1.555	1.062	1.016	3.888	3.842	759.8	12.25	0,872	0.0146
	Exptl. 2	1.517	1.114	1.066	4.098	4.050	794.3	12.74	0,916	0.0139
	3	1.56	0.90	0.85		2.87	920.	27.	0.87	0.017
	4	1,525	0.939		3.937		832.6			
$C^3\Delta_{\mathbf{w}}$	1	1,550	0.825	0.778	4, 130	4.085	780.1	13, 18	0,877	0.0146
	Exptl. 2	~1.5	0.907	0.861	4,306	4,255	750.	27.		
	3	1.55	0.67	0.61		3.11	958.		0.88	0.016
	4	1.522	0.703		4.173		858.6			
$A^3\Sigma_{\mu}^{\bullet}$	1	1,558	0.745	0.698	4,206	4.160	764.6	13.94	0,868	0.0151
	Exptl. 2	1,522	0.824	0.775	4.389	4, 340	799, 1	12, 16	0.911	0.0142
	3	1.56	0.61	0.55		3.16	943.	29.	0.87	0,017
	4	1,528	0.626		4.249		836.6			
B 3 Σ.	1	1,627	1,136	1.091	6,079	6,032	724.9	7.04	0,791	0.0077
B Zu	Exptl. 2	1.604	1.007	0.963	6. 173	6, 119	709.1		0. 791	
	3	1.68	0.30	0.363	0, 173	6. 01	593.	10.61 27.	0.819	0.0119 0.012
	4	1, 625	0.805	0.20	6.308	0.01	667.8	. 21.	0. 74	0.012
- 1										
23Σ.	2	2.069	0.511	0.479	6.699	6.638	537.0	13.73	0.490	0,0045
	1 3 4	2.00	0.38	0.33		5.94	872.	18.	0.53	-0.009
		2.101	0.314		6.798		482.6	,		
2 1 II.	3	1.620	1.111	1.005	8.411	8, 423	1626.4	163.67	0.819	0.0388
	3	1.57	0.84	0.69		8.13	2559.	65.	0.84	0.005
1 ¹ Δ,	1	1,631	0.905	0.862	8.570	8,521	705.6	9,59	0.788	0,0101
	3	1.70	0.20	0.17	0.0.0	8, 64	549.	35.	0.73	0.027
	1 3 4	1.648	0.556		8.794	0.0.	627.2			0.02.
2 1 A.			0.437	0.406		0.000		10 51	0.547	0.0100
2 4	1 3	1.961		100.00	9.031	8.968	499.5	13.51	0.547	0.0102
		1.88	0.14	0.10		8.71	597.	26.	0.60	0.015
1 Σ.	1 3	1,611	1,653	1.555	10,430	10.386	792.4	7.71	0.811	0.0092
	3	1.66	0.74	0.70		10.28	625.	-1.	0.76	0.022
	4	1,655	0.920		10.187		652.8			

 $^{^{\}mathrm{a}}$ All experimental values are taken from Ref. 2.

Tabular Data. A-14.7. Separated-atom energy levels of $\mathbf{0}_2$ given in eV relative to the $^3\mathrm{P}$ + $^3\mathrm{P}$ asymptote.

Separated-atom limit	This work	Experiment	SH	MG
¹ S + ¹ S	9.79	8.380	9.46	8. 05
$^{1}D + ^{1}S$	7.14	6.157	7.28	6.36
$^3P + ^1S$	4.88	4.190	4.73	4.02
$^{1}D + ^{1}D$	4, 51	3, 935	5, 10	4.67
$^3P + ^1D$	2.25	1.967	2.55	2.34

Tabular Data. A-14.8. Equilibrium constants for five new, weakly bound states of $\mathbf{0}_2$.

State	$R_{e}(\text{Å})$	$D_e(eV)$	$T_e(eV)$
1 ⁵ ∏€	1,996	0.228	4.746
2 3 II g	1.721	0.327	6.884
33 II.	1,922	0.147	7.072
1 1 A.	2.002	0.196	9.282
4 1 II.	1.952	0.428	11,667

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